

=> fil reg

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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FILE 'REGISTRY' ENTERED AT 13:45:45 ON 06 MAR 1999  
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DICTIONARY FILE UPDATES: 4 MAR 99 HIGHEST RN 220094-18-8

TSCA INFORMATION NOW CURRENT THROUGH JUNE 29, 1998

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

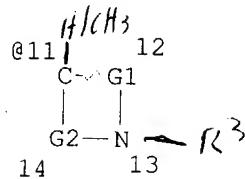
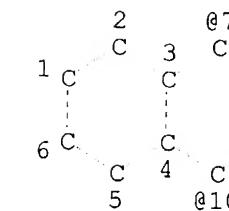
=> act berchnew522/a

L1 STR  
L2 STR  
L3 SEA FILE=REGISTRY SSS FUL L1 NOT L2

=> d 13 que stat

L1 STR

Buch cont



REP G1=(1-4) C  $\leftarrow$  Not subst  $\text{CH}_2 \text{ or } \text{CH}_3$

REP G2=(0-4) C  $\leftarrow$

VPA 11-7/8/9/10 U

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

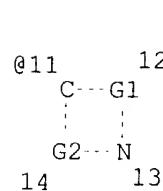
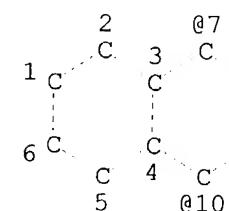
GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L2 STR



REP G1=(1-4) C

REP G2=(0-4) C

VPA 11-7/8/9/10 U

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L3 1213 SEA FILE=REGISTRY SSS FUL L1 NOT L2

100.0% PROCESSED 228041 ITERATIONS

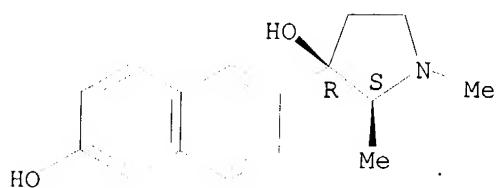
1213 ANSWERS

SEARCH TIME: 00.00.22

=> d scan

L3 1213 ANSWERS REGISTRY COPYRIGHT 1999 ACS  
IN 3-Pyrrolidinol, 3-(6-hydroxy-2-naphthalenyl)-1,2-dimethyl-,  
hydrochloride,  
monohydrate, (2S,3R)- (9CI)  
MF C16 H19 N O2 . Cl H . H2 O

Absolute stereochemistry. Rotation (-).

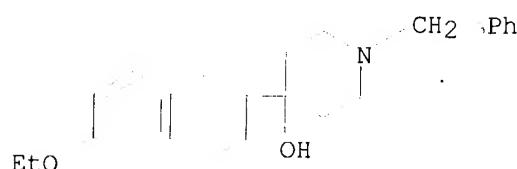


• HCl

• H2O

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):.

L3 1213 ANSWERS REGISTRY COPYRIGHT 1999 ACS  
IN 4-Piperidinol, 4-(6-ethoxy-2-naphthalenyl)-1-(phenylmethyl)- (9CI)  
MF C24 H27 N O2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> fil medline,capplus,biosis,embase;s 13

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
0.30	1136.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
	0.00	-4.82

FILE 'MEDLINE' ENTERED AT 13:46:19 ON 06 MAR 1999

FILE 'CAPLUS' ENTERED AT 13:46:19 ON 06 MAR 1999  
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L4	2	FILE MEDLINE
L5	416	FILE CAPLUS
L6	8	FILE BIOSIS
L7	1	FILE EMBASE

TOTAL FOR ALL FILES  
 L8 427 L3

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ENTER REMOVE, IDENTIFY, ONLY, OR (?):end

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PROCESSING COMPLETED FOR L8  
 L9 421 DUP REM L8 (6 DUPLICATES REMOVED)

=> d 1 100 200 300 400 421 cbib abs hitstr

L9 ANSWER 1 OF 421 CAPLUS COPYRIGHT 1999 ACS  
 1999:3260 Preparation and configuration of racemic and optically active analgesic cycloaminoalkylnaphthalenes. Ghislandi, Victor; Collina, Simona; Azzolina, Ornella; Barbieri, Annalisa; Lanza, Enrica; Tadini, Carla (Dipartimento di Chimica Farmaceutica, Universita di Pavia, Pavia, 27100, Italy). Chirality, 11(1), 21-28 (English) 1999. CODEN: CHRLEP. ISSN: 0899-0042. Publisher: Wiley-Liss, Inc..

AB Cycloaminoalkylnaphthalenes show interesting opioid-like analgesic properties. It possesses two chiral centers and can exist as two racemic pairs and four diastereomers. Since the binding of opioids with receptors

is stereoselective, it was important to have the two racemic pairs as well

as the four diastereomers. In this paper the synthesis of the (2R,3S/2S,3R) racemate and the (2R,3S) and (2S,3R) enantiomers of the 1,2-dimethyl-3-[2-(6-hydroxynaphthyl)]-3-hydroxypyrrolidine (I) is considered and the detn. of abs. configuration is described. The (2R,3S/2S,3R)-I racemate and the (2R,3S)-3 and (2S,3R)-I enantiomers were prep'd. by reaction of the racemic and optically active 1,2-dimethyl-3-pyrrolidone, resp., with the lithiation product obtained from 2-bromo-6-tetrahydropyranloxy-naphthalene and acidic hydrolysis. The above-mentioned enantiomers of I were also obtained by optical resoln.

HPT via fractional crystn. of the salts with D- and L-tartaric acids. The configuration of the optically active compds. was detd. by X-ray anal. of a crystal of  $(-)-(2S,3R)$ -I.cntdot.HCl.cntdot.H<sub>2</sub>O. The pharmacol. test

IT showed that  $(-)-(2S,3R)$ -I.cntdot.HCl.cntdot.H<sub>2</sub>O enantiomer is able to induce opioid-like analgesia with a relative potency 1.5 times that of  $(2R,3S/2S,3R)$ -I and .apprx.1.5 times that of morphine.

IT INDEXING IN PROGRESS

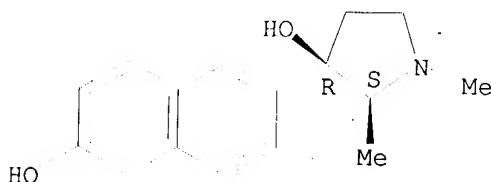
IT 210828-82-3P

RL: BAC (Biological activity or effector, except adverse); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. and configuration of racemic and optically active analgesic cycloaminoalkynaphthalenes)

RN 210828-82-3 CAPLUS

CN 3-Pyrrolidinol, 3-(6-hydroxy-2-naphthalenyl)-1,2-dimethyl-, hydrochloride, monohydrate,  $(2S,3R)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



• HCl

• H<sub>2</sub>O

IT 210828-78-7P

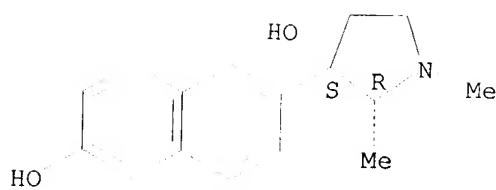
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant);

SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. and configuration of racemic and optically active analgesic cycloaminoalkynaphthalenes)

RN 210828-78-7 CAPLUS

CN 3-Pyrrolidinol, 3-(6-hydroxy-2-naphthalenyl)-1,2-dimethyl-, hydrochloride, monohydrate,  $(2R,3S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



• HCl

• H<sub>2</sub>O

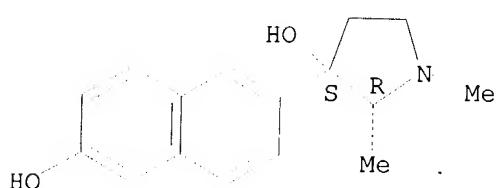
IT 210828-79-8P 210879-17-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and configuration of racemic and optically active analgesic  
cycloaminoalkynaphthalenes)

RN 210828-79-8 CAPLUS

CN 3-Pyrrolidinol, 3-(6-hydroxy-2-naphthalenyl)-1,2-dimethyl-, (2R,3S)-  
(9CI)  
(CA INDEX NAME)

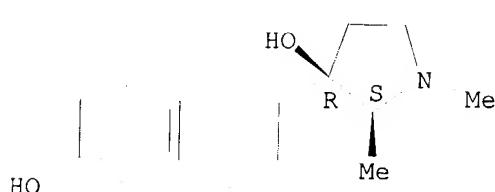
Absolute stereochemistry. Rotation (+).



RN 210879-17-7 CAPLUS

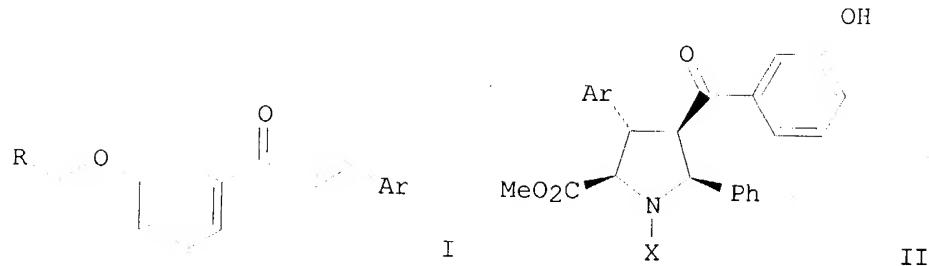
CN 3-Pyrrolidinol, 3-(6-hydroxy-2-naphthalenyl)-1,2-dimethyl-, (2S,3R)-  
(9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L9 ANSWER 100 OF 421 CAPLUS COPYRIGHT 1999 ACS

1997:10184 Document No. 126:144072 Stereoselective synthesis of highly  
functionalized pyrrolidines via 1,3-dipolar cycloaddition reactions on a  
solid support. Hollinshead, Sean P. (Sphinx Pharmaceuticals, A Division  
of Eli Lilly and Co., Durham, NC, 27707, USA). Tetrahedron Lett.,  
37(51),



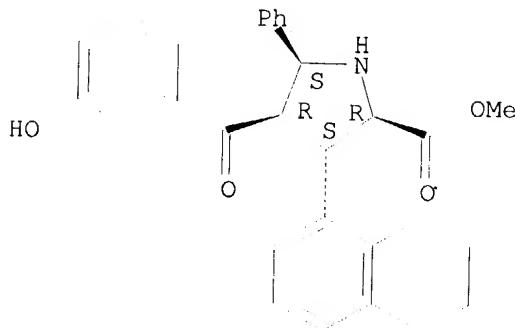
AB Resin bound 3-hydroxyacetophenone was condensed (NaOMe/MeOH/THF) with aryl aldehydes to give  $\alpha,\beta$ -unsatd. ketones. Subsequent reaction with an azomethine ylide in the presence of LiBr/DBU gave pyrrolidines. These pyrrolidines were subsequently acylated and cleaved from the solid support to give highly functionalized pyrrolidine target compds. Thus, the solid-supported 3-aryl-1-(3-hydroxyphenyl)-2-propen-1-ones I (R = methoxyphenyl, 1-naphthalenyl, etc.; R = resin support) were prep'd. Subsequent 1,3-dipolar cycloaddn. of I with N-benzylideneglycine Me ester gave the functionalized pyrrolidines II (same Ar; X = acyl, phenylsulfonyl group). Imines, such as N-[(4-methoxyphenyl)methylene]-3-pyridinemethanamine and N-[(4-bromophenyl)methylene]-3,4-dimethoxybenzenemethanamine did not undergo a dipolar cycloaddn. with I.

IT 186507-23-3DP, polymer-supported  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of pyrrolidines via 1,3-dipolar cycloaddn. on solid support)

RN 186507-23-3 CAPIUS

CN D-Proline, 4-(3-hydroxybenzoyl)-3-(1-naphthalenyl)-5-phenyl-, methyl ester, (3S,4R,5S)-rel- (9CI) (CA INDEX NAME)

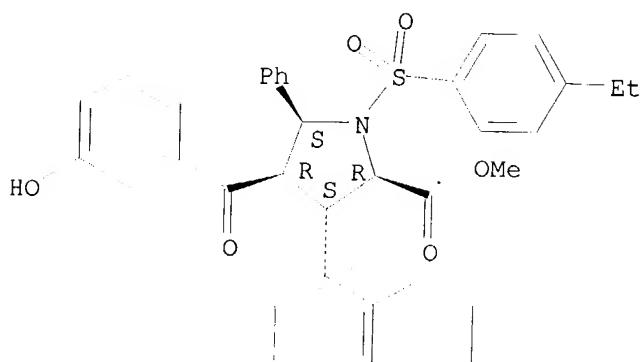
## Relative stereochemistry.



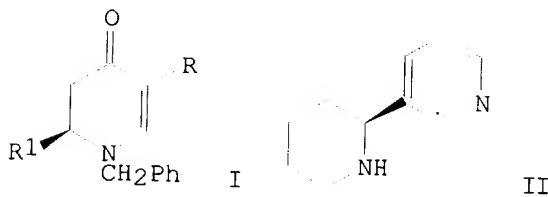
IT 186507-19-7P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of pyrrolidines via 1,3-dipolar cycloaddn. on solid support)  
RN 186507-19-7 CAPLUS

CN D-Proline, 1-[(4-ethylphenyl)sulfonyl]-4-(3-hydroxybenzoyl)-3-(1-naphthalenyl)-5-phenyl-, methyl ester, (3S,4R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L9 ANSWER 200 OF 421 CAPLUS COPYRIGHT 1999 ACS  
1992:408254 Document No. 117:8254 Asymmetric aza-Diels-Alder reaction  
mediated by chiral boron reagent. Hattori, Kouji; Yamamoto, Hisashi  
(Dep.  
Appl. Chem., Nagoya Univ., Nagoya, 464-01, Japan). J. Org. Chem.,  
57(12), 3264-5 (English) 1992. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES:  
CASREACT 117:8254; CJACS.  
GI



AB Asym. aza-Diels-Alder reaction of MeOCH:CRC(:CH<sub>2</sub>)OSiMe<sub>3</sub> (R = H, Me) with R1CH:NCH<sub>2</sub>Ph [R1 = Ph, 3-pyridyl, cyclohexyl, 3,5-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 2-naphthyl] mediated by a chiral complex generated in situ from (R)-binaphthyl and a triaryl borate gave the adducts I in high enantiomeric excess. The method

was used to prep. (-)-anabasine (II), using (S)-binaphthyl as the catalyst ligand.

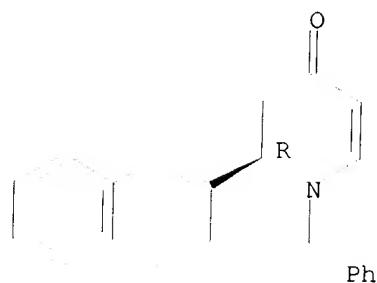
IT 141120-55-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(stereoselective prepn. of, catalysts for)

RN 141120-55-0 CAPLUS

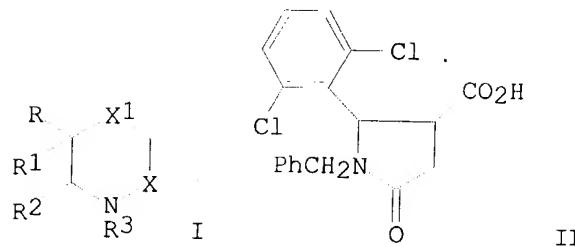
CN 4(1H)-Pyridinone, 2,3-dihydro-2-(2-naphthalenyl)-1-(phenylmethyl)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 300 OF 421 CAPLUS COPYRIGHT 1999 ACS  
 1985:78717 Document No. 102:78717 Analgesic 4-carboxy-pyrrolidin-2-one  
 compounds.. Shetty, Bola V.; McFadden, Arthur; Hofer, Peter (Purdue  
 Frederick Co., USA). U.S. US 4476311 A 19841009, 14 pp. Cont. of U.S.  
 Ser. No. 129,578, abandoned. (English). CODEN: USXXAM. APPLICATION: US  
 82-349992 19820219. PRIORITY: US 80-129578 19800312.

GI



AB Analgesic and antiinflammatory (no data) pyrrolidinecarboxylate derivs. I  
 (X = CO2CH2; X1 = bond, CH2, O, S; R = H, (un)substituted Ph; R1 = CH2OH,  
 carboxy, alkoxy, alkoxymethyl, aminomethyl, CH2CO2H; R2 = (un)substituted Ph,  
 naphthyl; R3 = Me, Et, Ph, CH2Ph, CH2CH2Ph] were prepd. Thus,  
 $2,6\text{-Cl}_2\text{C}_6\text{H}_3\text{CHO}$  and  $\text{H}_2\text{NCH}_2\text{Ph}$  gave 85%  $2,6\text{-Cl}_2\text{C}_6\text{H}_3\text{CH: NCH}_2\text{Ph}$ , which  
 underwent

cyclocondensation with succinic anhydride to give  
 pyrrolidinonecarboxylate

II.

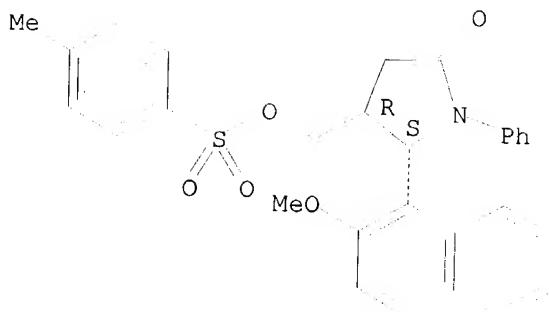
IT 94655-19-3P 94655-30-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and cyanation of)

RN 94655-19-3 CAPLUS

CN 2-Pyrrolidinone, 5-(2-methoxy-1-naphthalenyl)-4-[[[(4-methylphenyl)sulfonyl]oxy]methyl]-1-phenyl-, cis- (9CI) (CA INDEX NAME)

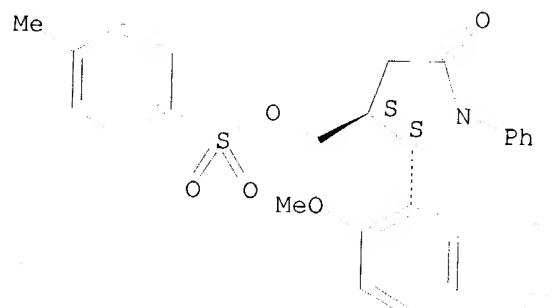
Relative stereochemistry.



RN 94655-30-8 CAPLUS

CN 2-Pyrrolidinone, 5-(2-methoxy-1-naphthalenyl)-4-[(4-methylphenyl)sulfonyl]oxy]methyl-1-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



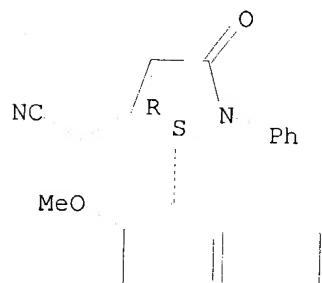
IT 94655-20-6P 94655-31-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and hydrolysis of)

RN 94655-20-6 CAPLUS

CN 3-Pyrrolidineacetonitrile, 2-(2-methoxy-1-naphthalenyl)-5-oxo-1-phenyl-, cis- (9CI) (CA INDEX NAME)

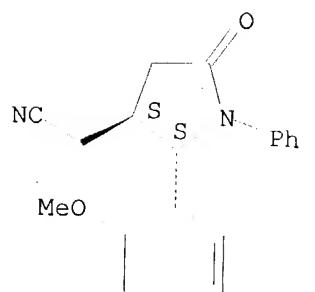
Relative stereochemistry.



RN 94655-31-9 CAPLUS

CN 3-Pyrrolidineacetonitrile, 2-(2-methoxy-1-naphthalenyl)-5-oxo-1-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



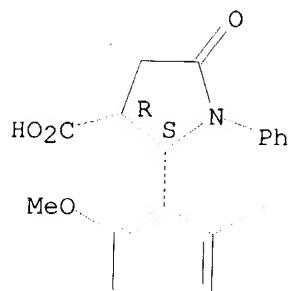
IT 94655-16-0P 94655-27-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and methylation of)

RN 94655-16-0 CAPLUS

CN 3-Pyrrolidinecarboxylic acid,  
2-(2-methoxy-1-naphthalenyl)-5-oxo-1-phenyl-  
, cis- (9CI) (CA INDEX NAME)

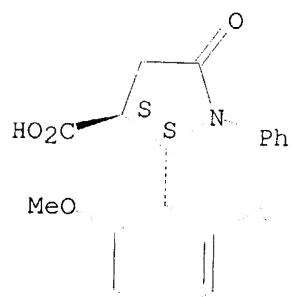
Relative stereochemistry.



RN 94655-27-3 CAPLUS

CN 3-Pyrrolidinecarboxylic acid,  
2-(2-methoxy-1-naphthalenyl)-5-oxo-1-phenyl-  
, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



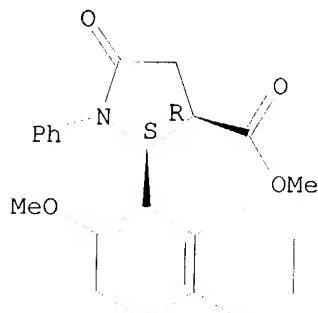
IT 94655-17-1P 94655-28-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and redn. of)

RN 94655-17-1 CAPLUS

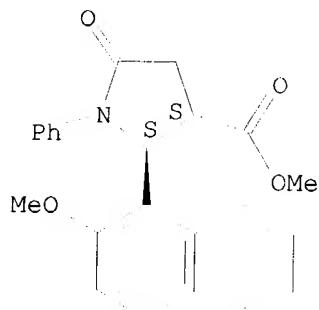
CN 3-Pyrrolidinecarboxylic acid,  
2-(2-methoxy-1-naphthalenyl)-5-oxo-1-phenyl-  
, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



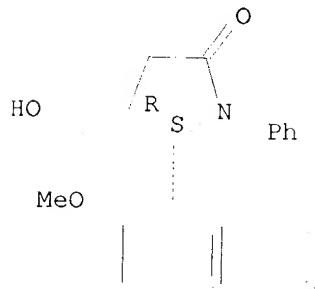
RN 94655-28-4 CAPLUS  
CN 3-Pyrrolidinecarboxylic acid,  
2-(2-methoxy-1-naphthalenyl)-5-oxo-1-phenyl-  
, methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 94655-18-2P 94655-29-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and tosylation of)  
RN 94655-18-2 CAPLUS  
CN 2-Pyrrolidinone,  
4-(hydroxymethyl)-5-(2-methoxy-1-naphthalenyl)-1-phenyl-,  
cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

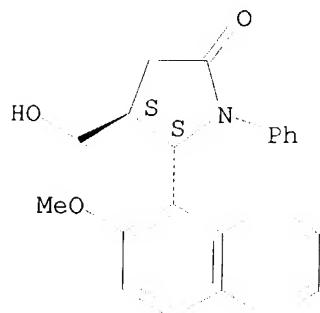


RN 94655-29-5 CAPLUS

CN 2-Pyrrolidinone,

4-(hydroxymethyl)-5-(2-methoxy-1-naphthalenyl)-1-phenyl-,  
trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



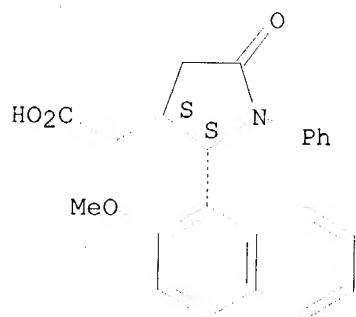
IT 94655-21-7P 94655-23-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 94655-21-7 CAPLUS

CN 3-Pyrrolidineacetic acid, 2-(2-methoxy-1-naphthalenyl)-5-oxo-1-phenyl-,  
cis- (9CI) (CA INDEX NAME)

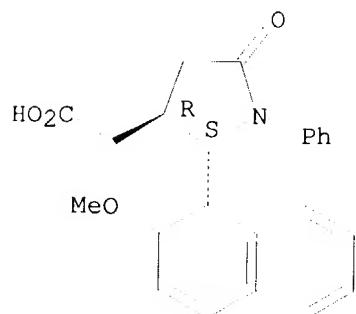
Relative stereochemistry.



RN 94655-23-9 CAPLUS

CN 3-Pyrrolidineacetic acid, 2-(2-methoxy-1-naphthalenyl)-5-oxo-1-phenyl-,  
trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L9 ANSWER 400 OF 421 CAPLUS COPYRIGHT 1999 ACS

1971:535519 Document No. 75:135519 Comparative studies of PMR spectra of some dihydropyridines. III. Kamal, A.; Begum, Tahira; Khan, M. Afzole; Qureshi, Asaf A. (Pakistan Counc. Sci. Ind. Res. Lab., Karachi, Pak.). Pak. J. Sci. Ind. Res. 14(1-2) 11-14 (English) 1971. CODEN: PGSNA

AB *J. Org. Chem.*, 36(12), 2111-2114 (English) 1971. CODEN: PSIRAA. The 60-MHz PMR spectra of a series of 4-substituted 2,6-dimethyl-3,5-bis(ethoxycarbonyl)-1,4-dihydropyridines in  $\text{Me}_2\text{SO}-\text{d}_6$  are presented and compared (substituent = Ph, 2-chlorophenyl, 3-hydroxyphenyl, 4-nitrophenyl, 3,4-dimethoxyphenyl, or  $\alpha$ -naphthyl).

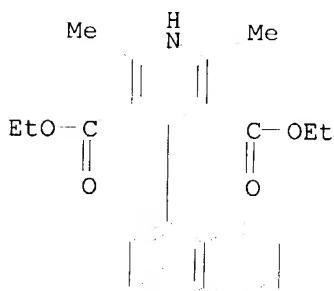
IT 34148-71-5

RL: PRP (Properties)  
(nuclear magnetic resonance of)

RN 34148-71-5 CAPLUS

CN 3,5-Pyridinedicarboxylic acid.

1,4-dihydro-2,6-dimethyl-4-(1-naphthalenyl)-  
, diethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 421 OF 421 CAPLUS COPYRIGHT 1999 ACS

1967:55380 Document No. 66:55380 Substituted pyrroles. Huisgen, Rolf (Union

Carbide Corp.). U.S. US 3285931 19661115, 9 pp. (English). CODEN: USXXXAM. APPLICATION: US 19641221.

GI For diagram(s), see printed CA Issue

AB The title compds. (I), which are useful as intermediates, are prep'd. from the reaction of an acetylenic compd.  $R_3C\text{-}C\equiv C\text{-}CR_4$  (II) with an azalactone (III) or mesoionic azalactone (IV) at 0-140. $^{\circ}$ ., where any R is H or an aliphatic, cycloaliphatic, aromatic, or heterocyclic function.

of 1-12 C's. It is also feasible to prep. III or IV in situ from amino acids with primary or secondary amino groups or the N-acyl derivs. with the aid of an acid anhydride. As an example, 1.75 g.

<sup>10</sup> *z*-phenyl-4-methyl-5-oxazolone is refluxed with 2.84 g. di-Me acetylene-dicarboxylate (V) in

ml. volume until concentration of 600 mg. per ml.

125-7.degree. (MeOH). VI is also obtained by using phenylglycine or N-acetylphenylglycine and Ac<sub>2</sub>O to generate the azalactone in situ. Similarly, 2,4-dihydro-1,3-dihydro-2H-1,2,4,5-tetrahydronaphthalene-1,2-dione is obtained by using 2,4-dihydro-1,3-dihydro-2H-1,2,4,5-tetrahydronaphthalene-1,2-diol and Ac<sub>2</sub>O.

Similarly, 2,4-diphenyloxazolone or N-benzoylphenylglycine with V gives (83% and 92% resp.) di-Me 2,5-diphenylpyrrole-3,4-dicarboxylate, m. 149-50° dec.  $\lambda_{\text{max}}$  250, 310, 360, 400, 420, 440, 460, 480, 500, 520, 540, 560, 580, 600, 620, 640, 660, 680, 700, 720, 740, 760, 780, 800, 820, 840, 860, 880, 900, 920, 940, 960, 980, 1000, 1020, 1040, 1060, 1080, 1100, 1120, 1140, 1160, 1180, 1200, 1220, 1240, 1260, 1280, 1300, 1320, 1340, 1360, 1380, 1400, 1420, 1440, 1460, 1480, 1500, 1520, 1540, 1560, 1580, 1600, 1620, 1640, 1660, 1680, 1700, 1720, 1740, 1760, 1780, 1800, 1820, 1840, 1860, 1880, 1900, 1920, 1940, 1960, 1980, 2000, 2020, 2040, 2060, 2080, 2100, 2120, 2140, 2160, 2180, 2200, 2220, 2240, 2260, 2280, 2300, 2320, 2340, 2360, 2380, 2400, 2420, 2440, 2460, 2480, 2500, 2520, 2540, 2560, 2580, 2600, 2620, 2640, 2660, 2680, 2700, 2720, 2740, 2760, 2780, 2800, 2820, 2840, 2860, 2880, 2900, 2920, 2940, 2960, 2980, 3000, 3020, 3040, 3060, 3080, 3100, 3120, 3140, 3160, 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149-50. degree.; 2-phenyl-4-[o-nitrophenyl]oxazolone with V gives 60% 2-[o-nitrophenyl]-5-phenylpyrroledicarboxylic acid 3,4-dimethyl

ester, m. 158-60. degree.; 2-[p-methoxyphenyl]-4-oxazolone with V gives 2-[p-methoxyphenyl]-5-phenylpyrroledicarboxylic acid 3,4-dimethyl ester.

oil; N-anisoylphenylglycine with V gives 98% di-Me 2-phenyl-5-[4-methoxyphenyl]pyrrole-3,4-dicarboxylate, b0.02 260-5.degree.; 2-phenyl-5-methyloxazolone or N-benzoylalanine with propiolic acid methyl ester (VII) give (98% for the latter) Me 2-phenyl-5-methylpyrrole-3(or 4)-carboxylate, b0.04 150-60.degree.; 2,4-diphenyloxazolone with VII gives

76% Me 2,5-diphenylpyrrole-3-carboxylate, m. 172-3.degree.; 2,4-diphenyl-5-oxazolone with 2-acetylphenylacetylene gives 12% 2,3,5-triphenyl-4-acetylpyrrole, m. 145-7.degree.; anhydro-5-hydroxy-3-methyl-2,4-diphenyloxazolium hydroxide (VIII) or N-benzoyl-N-methyl-phenylglycine (IX) with V give (95% and 92%, resp.) di-Me 2,5-diphenyl-1-methylpyrrole-3,4-dicarboxylate, m. 147-8.degree.; VIII or IX with phenylacetylene (X) give (66% and 93%, resp.) 2,3,5-triphenylpyrrole, m. 178-9.degree.; VIII or IX with diphenylacetylene give

(11% and 21%) 2,3,4,5-tetraphenyl-1-methylpyrrole, m., resp. 209-11.degree.; VIII or IX with Me propionate give (95% and 90%, resp.) Me

2,5-diphenyl-1-methylpyrrole-3-carboxylate, m. 99-100.degree.; IX with ethyl phenylpropionate (XI) gives 87% Et

2,3,5-triphenyl-1-methylpyrrole-4-carboxylate, m. 170-1.5.degree.; VIII with 1-hexyne gives 81% 2,5-diphenyl-1-methyl-3-butylpyrrole, b. 160-5.degree.; N-acetyl-N-phenylalanine (XII) with V gives 80% di-Me 1-phenyl-2,5-dimethylpyrrole-3,4-dicarboxylate, m. 87-8.degree.; XII with XI gives 88% Et 1,3-diphenyl-2,5-dimethylpyrrole-4-carboxylate, m. 77-9.degree.; XII with X gives 80% 1,3-diphenyl-2,5-dimethylpyrrole, oil, b0.001 150-70.degree.; N-benzoyl-N-methylalanine or N-acetyl-N-methylphenylglycine (XIII) with V give (83% and 90%, resp.) di-Me 2-phenyl-1,5-dimethylpyrrole-3,4-dicarboxylate, m. 94-5.degree.; XIII

with

XI gives 75% Et 1,2-dimethyl-3,5-diphenylpyrrole-4-carboxylate, m. 117-19.degree.; XIII with X gives 77% 1,2-dimethyl-3,5- or 1,2-dimethyl-4,5-diphenylpyrrole, m. 144-5.degree.; sarcosine with V gives

37% di-Me 1,2-dimethylpyrrole-3,4-dicarboxylate, m. 88-9.degree.; N-formyl-N-phenylglycine with V gives 92% di-Me 1-phenylpyrrole-3,4-dicarboxylate, m. 117-18.degree., L-proline with V gives 76% di-Me 1,2-dihydro-5-methyl-3H-pyrrolizine-6,7-dicarboxylate, m. 102-3.degree.; N-cyclohexylcarbonylphenylglycine with V gives 93% di-Me 2-cyclohexyl-5-phenyl-pyrrole-3,4-dicarboxylate, m. 143-5.degree.; N-(.alpha.-naphthoyl)phenyl glycine with V gives 85% di-Me 2-(.alpha.-naphthyl)-5-phenyl-pyrrole-3,4-dicarboxylate, m.

160-1.degree.;

N-(p-chlorobenzoyl)-phenylglycine with V gives 99.6% di-Me 2-phenyl-5-p-chlorophenylpyrrole-3,4-dicarboxylate, m. 143-4.degree.;

VIII

with acetylene gives 96% 2,5-diphenyl-1-methylpyrrole, m. 204-5.degree.; N-acetyl-N-phenylglycine with V gives 76% di-Me 1-phenyl-2-methylpyrrole-3,4-dicarboxylate, m. 66-8.degree.; N-methylalanine with V gives 87% di-Me

1,2,5-trimethylpyrrole-3,4-dicarboxylate m. 152-3.degree.;

N-cyclohexylcarbonyl-N-methylphenylglycine with V gives 98% di-Me 1-methyl-2-cyclohexyl-5-phenylpyrrole-3,4-dicarboxylate, m.

153-4.degree.;

N-acetyl-N-cyclohexylalanine with V gives 97% di-Me 2,5-dimethyl-1-cyclohexylpyrrole-3,4-dicarboxylate, m. 74-6.degree.; VIII with 1-benzoyl-2-phenylacetylene gives 68% 2,3,5-triphenyl-1-methyl-4-benzoylpyrrole, m. 214-15.degree.; DL-alanine with V gives 45% di-Me 2,5-dimethyl-3,4-bis-(methoxycarbonyl)pyrrole-1-maleate, m. 119-20.degree.; N-phenyl-acetylphenylalanine with V gives 11% di-Me

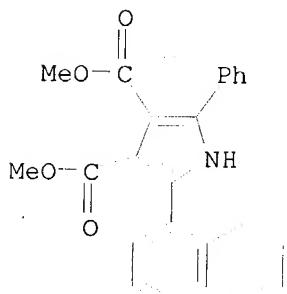
2,5-dibenzyl-3,4-bis(methoxycarbonyl)pyrrole-1-maleate, m. 137-8.degree.;  
 DL-phenylalanine with V gives 10.6% di-Me 2-methyl-5-benzyl-3,4-bis-(methoxycarbonyl)pyrrole-1-maleate, m. 131-2.degree.;  
 N-capronyl-DL-leucine with V gives 98% di-Me 2-n-amyl-5-(2-methylpropyl)-3,4-bis(methoxycarbonyl)pyrrole-1-maleate, b0.05 195-200.degree.;  
 L-tyrosine with V gives 39% di-Me 2-methyl-5-(4-acetoxyphenyl)-3,4-bis(methoxycarbonyl)pyrrole-1-maleate, m. 108-9.degree.; DL-tryptophan with V gives 52% di-Me 2-methyl-5-(.beta.-indolyl-methyl)-3,4-bis(methoxycarbonyl)pyrrole-1-maleate, m. 156-7.degree.;  
 N-isobutyryl-DL-valine with V gives 91% di-Me 2,5-diisopropyl-3,4-bis(methoxycarbonyl)pyrrole-1-maleate, oil, b0.005 180-5.degree..

IT 13712-62-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 13712-62-4 CAPLUS

CN Pyrrole-3,4-dicarboxylic acid, 2-(1-naphthyl)-5-phenyl-, dimethyl ester  
 (8CI) (CA INDEX NAME)



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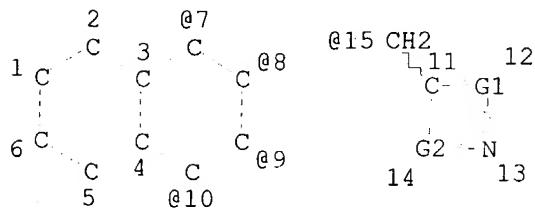
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REP G1=(1-4) C

REP G2=(0-4) C

VPA 15-7/8/9/10 U

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

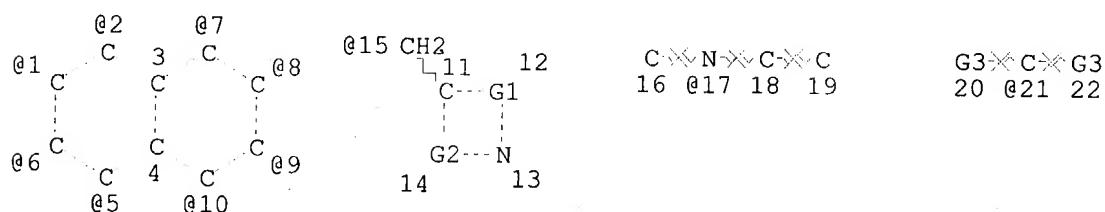
GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L11 STR



S---G4 G5 @25  
@23 24

REP G1=(1-4) C

REP G2=(0-4) C

VAR G3=C/N

VAR G4=H/ME

VAR G5=17/21/23/X

VPA 15-7/8/9/10 U

VPA 25-2/1/6/5 U

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L12 209 SEA FILE=REGISTRY SSS FUL L10 NOT L11

100.0% PROCESSED 218864 ITERATIONS

SEARCH TIME: 00.00.20

209 ANSWERS

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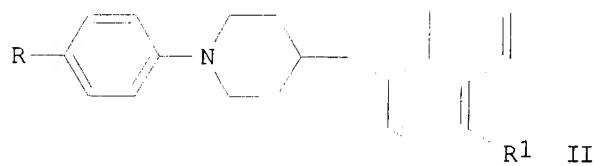
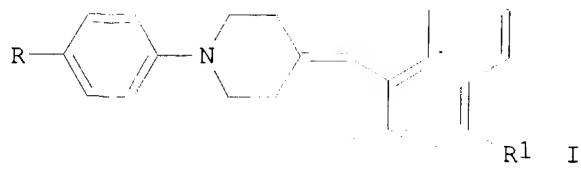
L13 0 FILE MEDLINE  
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 L15 0 FILE BIOSIS  
 L16 0 FILE EMBASE

TOTAL FOR ALL FILES  
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L17 ANSWER 1 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1998:739572 Document No. 130:52048 Exploring the limits of the  
 electrostatically induced conformational folding process in  
 charge-separated excited states. Retarding effect of long alkyl tails  
 attached to the chromophores. Lauteslager, Xavier Y.; Bartels, Marcel  
 J.;  
 Piet, Jacob J.; Warman, John M.; Verhoeven, Jan W.; Brouwer, Albert M.  
 (Institute Molecular Chemistry, University Amsterdam, Amsterdam, 1018 WS,  
 Neth.). Eur. J. Org. Chem. (11), 2467-2481 (English) 1998. CODEN:  
 EJOCFK. ISSN: 1434-193X. Publisher: Wiley-VCH Verlag GmbH.

GI



AB Six new donor-bridge-acceptor compds. were synthesized which contain a long n-tetradecyl chain attached to the donor or acceptor moiety, or to both of them. Compds. I (R = C<sub>14</sub>H<sub>29</sub>, R<sup>1</sup> = COOC<sub>14</sub>H<sub>29</sub>; R = Me, R<sup>1</sup> = COOC<sub>14</sub>H<sub>29</sub>; R = C<sub>14</sub>H<sub>29</sub>, R<sup>1</sup> = CN) are analogs of the fluorescent probe mol. Fluoroprobe. They contain a rigidly extended 4-methylenepiperidine bridge

and show relatively strong charge transfer fluorescence in solvents of low and medium polarity. Compds. II (R = C<sub>14</sub>H<sub>29</sub>; R<sup>1</sup> = COOC<sub>14</sub>H<sub>29</sub>; R = Me, R<sup>1</sup> =

= COOC<sub>14</sub>H<sub>29</sub>; R = C<sub>14</sub>H<sub>29</sub>, R<sup>1</sup> = CN) contain a semiflexible 4-methylpiperidine bridge, obtained after hydrogenation of the exocyclic double bond of I. These systems undergo a conformational change following photoinduced charge sepn. (harpooning) in nonpolar solvents and probably also in solvents of medium polarity. Both the steady-state fluorescence spectra and the fluorescence decay times of the extended charge transfer (ECT) species show that the photoinduced folding process is effectively slowed down by the introduction of the long alkyl tails. This is most pronounced

for II (R = C<sub>14</sub>H<sub>29</sub>; R<sup>1</sup> = COOC<sub>14</sub>H<sub>29</sub>) which has an n-tetradecyl group attached to both donor and acceptor. In soln. a small difference in the rate of folding is obsd. between II (R = Me, R<sup>1</sup> = COOC<sub>14</sub>H<sub>29</sub>; R = C<sub>14</sub>H<sub>29</sub>, R<sup>1</sup> = CN) which have a single n-tetradecyl chain attached to the acceptor only and to the donor only, resp.

L17 ANSWER 2 OF 94 CAPLUS COPYRIGHT 1999 ACS

1998:482484 Document No. 129:216203 First asymmetric nucleophilic displacement reactions on chiral .alpha.-substituted aldehyde hydrazones. Enders, Dieter; Maassen, Ralf; Rumsink, Jan (Institut fur Organische Chemie, Rheinisch Westfälische Technische Hochschule, Aachen, D-52074, Germany). Tetrahedron: Asymmetry, 9(12), 2155-2180 (English) 1998. CODEN: TASYE3. ISSN: 0957-4166. OTHER SOURCES: CASREACT 129:216203. Publisher: Elsevier Science Ltd..

AB The first asym. nucleophilic substitution reactions on racemic .alpha.-substituted aldehydes using enantiomerically pure hydrazines as chiral auxiliaries is presented. The diastereoselectivity of the process is achieved by a dynamic kinetic resln. via the 1:1 epimeric mixt. of the substrate hydrazones. The a<sub>2</sub>-reactivity (Umpolung) of the .alpha.-substituted hydrazones is accomplished by complexation with Lewis

acids. Several carbon, sulfur and oxygen nucleophiles were shown to readily undergo substitution of the  $\alpha$ -leaving group under these conditions, affording the substitution products with good to excellent chem. yields and with low to moderate diastereoselectivities. Two methods

for cleavage of the chiral auxiliary are described.

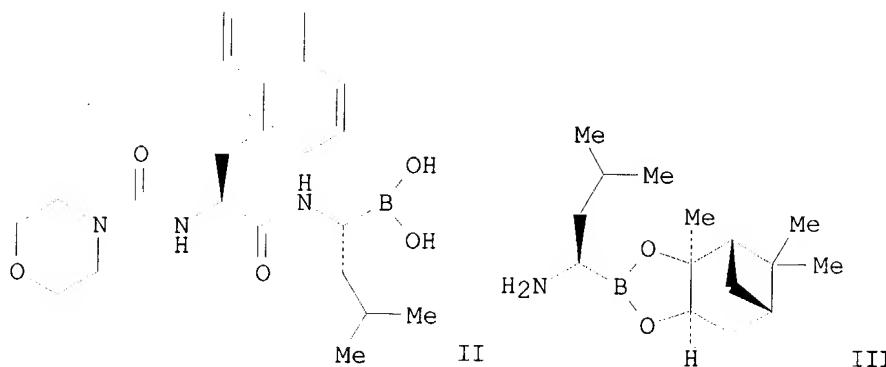
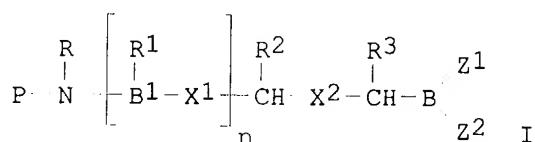
L17 ANSWER 3 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1998:479021 Document No. 129:122868 Preparation of peptidylboronic ester and

acid compounds as proteasome inhibitors. Adams, Julian; Ma, Yu-Ting; Stein, Ross; Baevsky, Matthew; Grenier, Louis; Plamondon, Louis (Proscript, Inc., USA). U.S. US 5780454 A 19980714, 37 pp.

Cont.-in-part

of U.S. Ser. No. 442,581. (English). CODEN: USXXAM. APPLICATION: US 95-549318 19951027. PRIORITY: US 94-330525 19941028; US 95-442581 19950516.

GI



AB Disclosed herein is a method for reducing the rate of degrdn. of proteins in an animal comprising contacting cells of the animal with certain boronic ester and acid compds I [P = aryl-, aralkyl-, heteroaryl-, or heteroarylalkylcarbonyl or -sulfonyl; B1 = N, CH; X1, X2 = CONH, CH(OH)CH2, COCH2; n = 0, 1, 2; R = H, alkyl; RR1 or RR2 (for n = 0) may form a ring; R1, R2, R3 = H, alkyl, cycloalkyl, aryl, etc.; Z1, Z2 = alkyl, hydroxy, alkoxy, aryloxy; Z1Z2 may form a moiety derived from a dihydroxy compd.]. Also disclosed herein are novel boronic ester and acid compds., their synthesis and uses. Thus, peptidylboronic acid II was prep'd. by coupling pinanediol leucine boronate ester III with N-Boc- $\beta$ -(1-naphthyl)-L-alanine, followed by deprotection, acylation with 4-morpholinecarbonyl chloride, and cleavage of the pinanediol moiety.

II inhibited proteasome 20S wth Ki = 0.18 nM.

L17 ANSWER 4 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1998:296813 Document No. 129:33967 Femtosecond solvation and charge transfer  
dynamics in liquid solution. Glasbeek, M. (Laboratory for Physical Chemistry, University of Amsterdam, Amsterdam, 1018 WS, Neth.). Czech. J. Phys., 48(4), 417-422 (English) 1998. CODEN: CZYPAO. ISSN: 0011-4626. Publisher: Institute of Physics, Academy of Sciences of the Czech Republic.

AB Time-resolved fluorescence up-conversion expts. were performed for a few fluorescent org. charge transfer mols. in liq. soln. Dynamic Stokes shifts were measured, with a time resoln. of 150 fs, for the probe mols. in alc. and ethereal solvents. The results reveal solvation dynamics detd. by inertial free streaming motions of the solvent mols. in the solvent cages and rotational diffusion motions of the solvent mols. Simulations of the temporal changes in the fluorescence spectra based on the Smoluchowski diffusion equation are also briefly discussed.

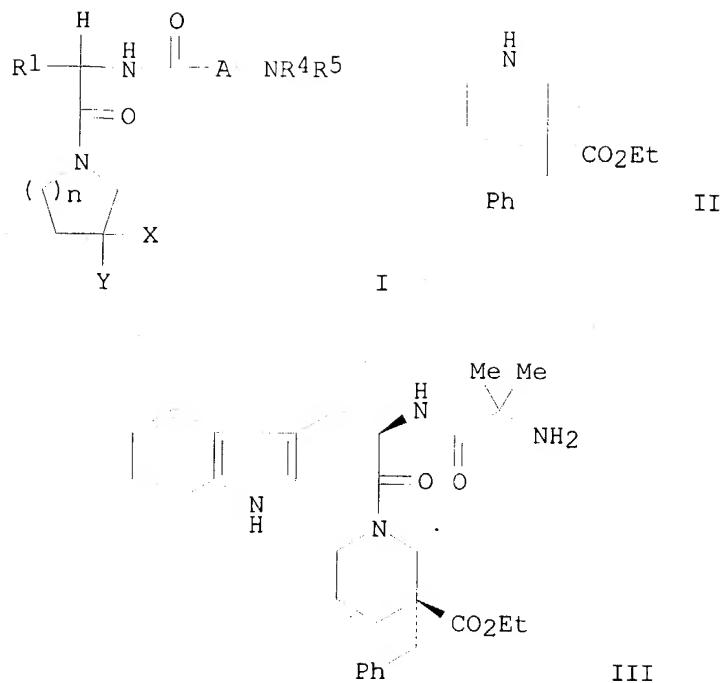
L17 ANSWER 5 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1998:213073 Document No. 128:270554 Preparation of 7-arylmethyl-1H-pyrrolo[3,4-c]pyridine-1,3-(2H)-diones and .alpha.-aryl-3-hydroxy-5-pyridylacetonitriles using arynic methodology. Wang, Anlai; Tandel, Sagun; Zhang, Hongming; Huang, Yuwei; Holdeman, Terra C.; Biehl, Edward R. (Chemistry Department, Southern Methodist University, Dallas, TX, 75275, USA). Tetrahedron, 54(14), 3391-3400 (English) 1998. CODEN: TETRAB. ISSN: 0040-4020. Publisher: Elsevier Science Ltd..

AB 7-Arylmethyl-1H-pyrrolo[3,4-c]pyridine-1,3-(2H)-diones and .alpha.-aryl-3-hydroxy-5-pyridylacetonitriles can be prepd. in modest yields from the resp. reactions of 5-bromonicotinamide and 5-chloro-3-pyridinol with arylacetonitriles and LDA.

L17 ANSWER 6 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1998:146698 Document No. 128:205144 Di- and trisubstituted piperidine, pyrrolidine and hexahydro-1H-azepine peptide analogs promote release of growth hormone. Morriello, Gregori J.; Yang, Lihu; Patchett, Arthur A. (Merck and Co., Inc., USA). U.S. US 5721250 A 19980224, 81 pp. Cont.-in-part of U.S. 5,492,916. (English). CODEN: USXXAM.

APPLICATION:  
US 96-600646 19960213. PRIORITY: US 93-173449 19931223; US 94-323988 19941017.

GI



AB The present invention is directed to certain novel compds. identified as di- and trisubstituted piperidines, pyrrolidines and hexahydro-1H-azepines of the general structural I [R1 = e.g., C1-10 alkyl, aryl, aryl(C1-6 alkyl); X = e.g., H, CN,  $(CH_2)_qNR_2COR_2$ ,  $(CH_2)_qNR_2SO_2(CH_2)paryl$ ,  $(CH_2)_qNR_2SO_2R_2$ ; Y = e.g., H, C1-10 alkyl,  $(CH_2)paryl$ ; R2 = e.g., H, C1-6 alkyl, C3-7 cycloalkyl; q = 0-4; p = 0-3; R4, R5 = independently, e.g., H, C1-6 alkyl; A =  $(CH_2)_xCR_7R_7a(CH_2)_y$ , Z $(CH_2)_xCR_7R_7a(CH_2)_y$ ; x, y = independently 0-3; Z = NR6a, O; R6a = H, C1-6 alkyl; R7, R7a = independently, e.g., H, C1-6 alkyl, CF3; n = 1-3]. These compds. promote the release of growth hormone in humans and animals (no data). This property can be utilized to promote the growth of food animals to render the prodn. of edible meat products more efficient, and in humans, to treat physiol. or medical conditions characterized by a deficiency in growth hormone secretion, such as short stature in growth hormone deficient children, and to treat medical conditions which are improved by the anabolic effects of growth hormone. Growth hormone releasing compns. contg. such compds. as the active ingredient thereof are also disclosed. Thus, e.g., amide coupling of benzylpiperidinecarboxylate II.HCl (prepn. given) with Boc-D-Trp-OH (Boc = Me<sub>3</sub>CO<sub>2</sub>C) acid followed by deprotection and coupling with N-Boc-.alpha.-methylalanine and deprotection afforded piperidine deriv. III.HCl.

L17 ANSWER 7 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1997:750000 Document No. 128:75261 Synthesis of 1,2,3,5-substituted  
pyrroles through palladium-catalyzed reaction of ethyl 2-acetyl-4-pentynoate  
tosylhydrazone with aryl iodides. Arcadi, Antonio; Anacardio, Roberto;  
D'Anniballe, Gaetano; Gentile, Marco (Departimento Chimica Ingegneria  
Chimica Materiali, Facolta Scienze, Universita L'Aquila, L'Aquila,

I-67100, Italy). *Synlett* (11), 1315-1317 (English) 1997. CODEN: SYNLES. ISSN: 0936-5214. OTHER SOURCES: CASREACT 128:75261. Publisher: Georg Thieme Verlag.

AB The reaction of 2-acetyl-4-pentyneoate tosylhydrazone with aryl iodides in the presence of  $K_2CO_3$  and catalytic amounts of a Pd complex affords 1-(tosylamino)-2-methyl-5-(aryl methyl)-3-pyrrolecarboxylates in satisfactory yield.

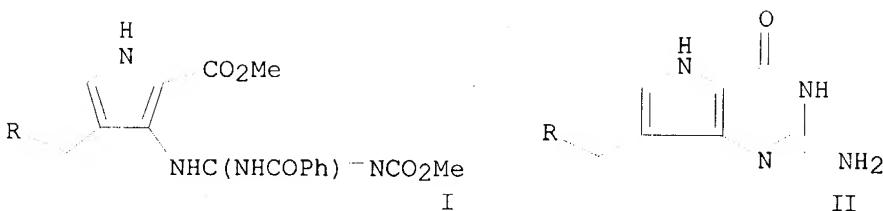
L17 ANSWER 8 OF 94 CAPLUS COPYRIGHT 1999 ACS

1997:720363 Document No. 127:331453 An Improved Synthesis of 7-Substituted Pyrrolo[3,2-d]pyrimidines. Elliott, Arthur J.; Morris, Philip E., Jr.; Petty, Sandra L.; Williams, Carl H. (BioCryst Pharmaceuticals Inc., Birmingham, AL, 35244, USA). J. Org. Chem., 62(23), 8071-8075 (English) 1997. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CJACS.

Publisher:

American Chemical Society.

GT



AB Base-catalyzed condensation of 3,3-dimethoxypropionitrile with RCHO [R = (un)substituted Ph, naphthyl, cyclohexyl, 2-furyl, 3-thienyl] followed by hydrolysis with 6 N HCl gives RCH:C(CN)CHO. Catalytic redn. of the double bond followed by reaction with di-Et aminomalonate affords RCH<sub>2</sub>C(CN):CHNHCH(CO<sub>2</sub>Et)<sub>2</sub>, which cyclize to aminopyrroles on treatment with NaOMe. While the amino group in these compds. is unreactive toward many guanylating reagents, acid-catalyzed guanylation occurs easily with MeO<sub>2</sub>CN:C(SMe)NHCO<sub>2</sub>Me to give pyrroles I. Subsequent facile removal of the carbamate groups and ring closure to the pyrrolo[3,2-d]pyrimidine ring system II occurs on treatment with base. The use of HgCl<sub>2</sub> in place of AcOH ties up the mercaptan and eliminates the odor problem. For larger scale reactions where the mercaptan odor and the use of Hg salts are undesirable, the use of MeO<sub>2</sub>CN:C(OMe)NHCO<sub>2</sub>Me is preferred. Using this procedure, II [R = Ph], a potent inhibitor of the enzyme purine nucleoside phosphorylase, was prep'd. in 31% overall yield with only three isolation steps.

L17 ANSWER 9 OF 94 CAPLUS COPYRIGHT 1999 ACS

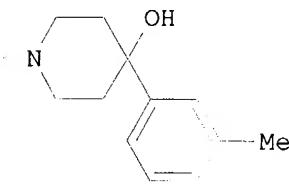
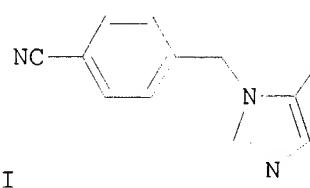
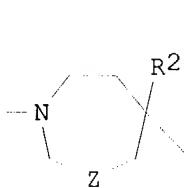
1997:696612 Document No. 127:358860 Preparation of 1-(4-cyanobenzyl)-5-piperidinomethylimidazoles as farnesyl protein transferase inhibitors. Anthony, Neville J.; Dinsmore, Christopher; Gomez, Robert P.; Hutchinson, John H.; Wai, John S.; Williams, Theresa M.; Bell, Ian M.; Embrey, Mark W.; Fisher, Thorsten E. (Merck & Co., Inc., USA; Anthony, Neville J.; Dinsmore, Christopher; Gomez, Robert P.; Hutchinson, John H.; Wai, John S.; Williams, Theresa M.; Bell, Ian M.; Embrey, Mark W.; Fisher, Thorsten

E.). PCT Int. Appl. WO 9738665 A2 19971023, 326 pp. DESIGNATED STATES: W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 97-US6487 19970327.

PRIORITY:

US 96-14791 19960403; GB 96-9981 19960513.

GI



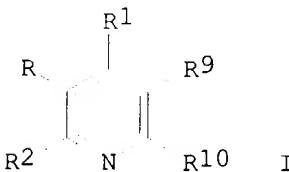
II

AB RA1[C(R1a)2]nA2[C(R1a)2]nZ1[C(R1b)2]pXZ2X1[C(R1c)2]vR1 [I; A1,A2 = bond, CH:CH, CO, O, (alkyl)imino, etc.; R = H, (un)substituted heterocyclyl, -aryl, etc.; R1 = (un)substituted heterocyclyl or -aryl; R1a,R1b = H, OH, alkyl, alkoxy, aryl, etc.; R1c = H, alkyl, aryl, etc.; X = bond, CH2, CO, etc.; X1 = bond, CH2, CO, O, etc.; Z1 = (un)substituted heterocyclylene; Z2 = azacycloalkylene group I; R2 = H, hydroxy(alkyl), alkoxy(alkyl), alkyl, etc.; Z = bond or CH2; p,n = 0-4; v = 0-2] were prep'd. Thus, 1-(4-cyanobenzyl)-5-imidazolecarboxaldehyde was reductively aminated by 4-(3-methylphenyl)-4-hydroxypiperidine (prepn. each given) to give title compd. II. Data for biol. activity of I were given.

L17 ANSWER 10 OF 94 CAPLUS COPYRIGHT 1999 ACS

1997:667709 Document No. 127:307306 Preparation of 2-arylpyridine-3-methanols and analogs as cholesteryl ester transfer protein inhibitors. Schmidt, Gunter; Angerbauer, Rolf; Brandes, Arndt; Loegers, Michael; Mueller-gliemann, Matthias; Bischoff, Hilmar; Schmidt, Delf; Wohlfeil, Stefan (Bayer A.-G., Germany). Eur. Pat. Appl. EP 796846 A1 19970924, 59 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE. (German). CODEN: EPXXDW. APPLICATION: EP 97-103813 19970307. PRIORITY: DE 96-19610932 19960320.

GI



AB Title compds. [I; R = hydroxyalkyl; R1,R2 = (un)substituted aryl; R9 = ZR3 or CR4R5R6; R3,R4 = cycloalkyl, aryl, heterocyclyl, etc.; R5 = H and R6 = H, halo, alkoxy, (di)(alkyl)amino, etc.; R5R6 = O; R6 = H, halo, OH, etc.]; R10 = (cyclo)alkyl; Z = (hydroxy- or halo-substituted) alk(en)ylene] were prep'd. Thus, Me2CHC(NH2):CHCO2Et was cyclocondensed with 4-FC6H4CHO and

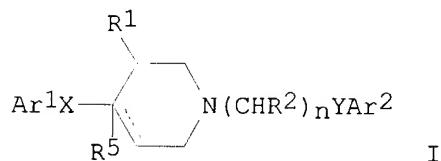
4-FC<sub>6</sub>H<sub>4</sub>COCH<sub>2</sub>CO<sub>2</sub>Me and the dehydrogenated product reduced to give I (R<sub>1</sub> = R<sub>2</sub> = C<sub>6</sub>H<sub>4</sub>F-4, R<sub>10</sub> = CHMe<sub>2</sub>) (II; R = CO<sub>2</sub>Me, R<sub>9</sub> = CH<sub>2</sub>OH) which was oxidized and the product condensed with 4-(F<sub>2</sub>C)C<sub>6</sub>H<sub>4</sub>Br/Mg to give, after redn., II [R = CH<sub>2</sub>OH, R<sub>9</sub> = CH(OH)C<sub>6</sub>H<sub>4</sub>(CF<sub>3</sub>)-4]. Data for biol. activity of I were given.

L17 ANSWER 11 OF 94 CAPLUS COPYRIGHT 1999 ACS

1997:503392 Document No. 127:149079 Preparation of 4-substituted piperidine analogs and their use as subtype selective NMDA receptor antagonists. Bigge, Christopher F.; Cai, Sui Xiong; Weber, Eckard; Woodward, Richard; Keana, John F. W.; Lan, Nancy C.; Guzikowski, Anthony P.; Zhou, Zhang-Lin;

Yeun, Po-Wai (Warner-Lambert Company, USA; Cogensys, Inc.; Bigge, Christopher F.; Cai, Sui Xiong; Weber, Eckard; Woodward, Richard; Keana, John F. W.; Lan, Nancy C.; Guzikowski, Anthony P.; et al.). PCT Int. Appl. WO 9723216 A1 19970703, 280 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 96-US20872 19961220. PRIORITY: US 95-9184 19951222.

GI



AB 4-Substituted piperidine analogs I [Ar<sub>1</sub>, Ar<sub>2</sub> = aryl, heteroaryl; X = (CHR<sub>3</sub>)<sub>m</sub>, O, S, NR<sub>4</sub>; R<sub>3</sub> = H, OH, alkyl; R<sub>4</sub> = H, alkyl; m = 0, 1, 2; R<sub>1</sub> = H, OH, alkyl; n = 0-4; Y = O, S, NR<sub>4</sub>, or a single bond; R<sub>5</sub> = H, OH; the dotted bond is a single or double bond] were prep'd. as selective active antagonists of N-methyl-D-aspartate (NMDA) receptor subtypes. E.g., reaction of 4-benzylpiperidine and 1-bromo-2-phenoxyethane gave 4-benzyl-1-(2-phenoxyethyl)piperidine. Data show that I exhibit selectivity for 2B subtype receptors compared to 2A and 2C subtype receptors. Many of the compds. are active as anticonvulsants. I also show significant protection from ischemia.

L17 ANSWER 12 OF 94 CAPLUS COPYRIGHT 1999 ACS

1997:348323 Document No. 127:81757 The solid phase synthesis of .alpha.,.alpha.-disubstituted unnatural amino acids and peptides (di-UPS).

Scott, William L.; Zhou, Changyou; Fang, Zhiqiang; O'Donnell, Martin J. (Res. Technologies Proteins, Lilly Res. Labs., Indianapolis, IN, 46285, USA). Tetrahedron Lett., 38(21), 3695-3698 (English) 1997. CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT 127:81757. Publisher: Elsevier.

AB This paper reports a new, mild procedure (di-UPS) for the solid phase synthesis of racemic .alpha.,.alpha.-disubstituted amino acids and epimeric .alpha.,.alpha.-disubstituted terminal amino acid residues in a resin-bound peptide. The synthetic route is compatible with most protected amino acid side chains and can be used in a continuing solid

phase synthesis. Di-UPS should find a wide applicability in the design and solid phase synthesis of hybrid amino acids and peptides and the construction of basis units for combinational chem.

L17 ANSWER 13 OF 94 CAPLUS COPYRIGHT 1999 ACS

1997:320514 Document No. 127:57847 Influence of solvent viscosity and permittivity on the harpooning mechanism in semirigidly bridged electron donor-acceptor systems. Jaeger, W.; Schneider, S.; Verhoeven, J. W. (Institute for Physical und Theoretical Chemistry, Friedrich-Alexander-Universitaet, Egerlandstr. 3, D-91058, Erlangen, Germany). Chem. Phys. Lett., 270(1,2), 50-58 (English) 1997. CODEN: CHPLBC. ISSN: 0009-2614. Publisher: Elsevier.

AB After the photoinduced electron transfer, the donor-bridge-acceptor system

"WS4" (1-Phenyl-4-[(4-cyano-1-naphthyl)methyl]piperidine) executes a large

scale motion which leads from an extended to a compact geometry (harpooning mechanism). The rate of this folding process,  $k_{fold}$ , was measured in three nonpolar solvents as a function of temp. (283 < T < 343 K) and hydrostatic pressure (0.1 < P < 350 MPa) and successfully fitted by the expression  $k_{fold} = B \cdot \text{cntdot.} (A/\eta) \cdot 0.7 \exp[-(Ester-E'')/\epsilon \cdot r + E''/\epsilon \cdot r^2]/RT]$ . This implies that the effect of friction on the folding kinetics of WS4 is modeled best by the same stretched exponential, in contrast to the previously studied structurally related systems WS2 and WS3 where no friction dependence was obsd.

L17 ANSWER 14 OF 94 CAPLUS COPYRIGHT 1999 ACS

1997:49616 Document No. 126:157370 SAR of 2-benzyl-4-aminopiperidines NK1 antagonists. Part 2. Synthesis of CGP 49823. Veenstra, Siem J.; Hauser, Kathleen; Schilling, Walter; Betschart, Claudia; Ofner, Silvio (Research Department, CIBA-GEIGY AG, Basel, CH-4002, Switz.). Bioorg. Med. Chem. Lett., 6(24), 3029-3034 (English) 1996. CODEN: BMCLE8. ISSN: 0960-894X. Publisher: Elsevier.

AB CGP 49823 is a potent NK1 antagonist which is centrally active after oral administration. The SAR of the C-2 substituent was investigated with respect to the affinity to the NK1 receptor. A practical synthesis of

CGP

49823, suitable for scale-up, was developed. The key-step, a tandem acyliminium ion cyclization/Ritter reaction, gave trans 2-benzyl-4-acetamidopiperidines with high diastereoselectivity.

L17 ANSWER 15 OF 94 CAPLUS COPYRIGHT 1999 ACS

1997:39263 Document No. 126:144541 Preparation of amino acid pharmaceuticals. Carrera, Jesus E.; Esteban, Almudena R.; Mann, Andre; Schoenfelder, Angele; Schoepp, Darryle D.; Tercero, Concepcion P.; Wermuth, Camille-Georges (Eli Lilly and Company, USA; Universite Louis Pasteur; Lilly, S.A.). U.S. US 5589501 A 19961231, 10 pp. (English). CODEN: USXXAM. APPLICATION: US 94-343817 19941122.

AB Amino acids  $R_1(CH_2)qCH:CH(CH_2)nCHR(CH_2)mCH(NH_2)CO_2H$  [R = CO<sub>2</sub>H, tetrazolyl;

$R_1 = (\text{un})\text{substituted Ph, naphthyl, thiienyl, etc.}; m = 0-2; n, q = 0-5; p$

=

0, 1] and their salts and esters were prep'd. for use as pharmaceuticals. The amino acids possess affinity for metabotropic glutamate receptors (formulations given). Thus, (2R,4R/S)-2-amino-4-(3'-phenyl-2'-propenyl)-1,5-pentanedioic acid was prep'd. from (4R)-1,1-dimethylethyl 4-(3'-ethoxy-3'-oxopropenyl)-2,2-dimethyl-3-oxazolidinecarboxylate via catalytic hydrogenation, alkylation with cinnamyl bromide, oxazolidine ring cleavage by pyridinium tosylate, oxidn. by pyridinium dichromate, esterification with diazomethane, and sapon.

L17 ANSWER 16 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1996:695117 Document No. 126:96278 Subpicosecond studies of the solvation dynamics of fluoroprobe in liquid solution. Middelhoek, E. R.; Zhang, H.;

Verhoeven, J. W.; Glasbeek, M. (Lab. Phys. Chem., Univ. Amsterdam, Amsterdam, 1018 WS, Neth.). Chem. Phys., 211(1,2,3), 489-497 (English) 1996. CODEN: CMPHC2. ISSN: 0301-0104. Publisher: Elsevier.

AB The dynamic Stokes shift of a fluoroprobe in its lowest excited charge transfer state was studied in solvents, at room temp., with a time resoln.

of .apprx.300 fs. Using the fluorescent upconversion method dynamic Stokes shifts of up to 3000 cm<sup>-1</sup> were resolved. The Stokes shift is attributed to the solvent response to the large photoinduced dipole moment

of fluoroprobe (.apprx.30 D) in the fluorescent charge transfer state. The solvation dynamics is detd. by the rotational diffusional motions of the ether solvent mols.

L17 ANSWER 17 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1996:538176 Document No. 126:110881 Suppression of the harpooning mechanism in donor-bridge-acceptor systems by aza substitution in the bridge. Lauteslager, Xavier Y.; Wegewijs, Bas; Verhoeven, Jan W.; Brouwer, Albert M. (Laboratory of Organic Chemistry, Amsterdam Institute of Molecular Studies, University of Amsterdam, Nieuwe Achtergracht 129, NL-1018 WS, Amsterdam, Neth.). J. Photochem. Photobiol., A, 98(3), 121-126 (English) 1996. CODEN: JPPCEJ. ISSN: 1010-6030. Publisher: Elsevier.

AB An aza substituent was introduced in the bridge of donor-bridge-acceptor systems known to undergo harpooning (long-range photoinduced charge sepn. followed by electrostatically driven folding). Although the substitution does not reduce the conformational flexibility of the bridge, it fully suppresses the harpooning mechanism. From a comparison with a ref. compd., the solvatochromic shifts of charge transfer fluorescence and transient absorption results, it is concluded that suppression is due to the low ionization potential of the aza substituent, which leads to a strong redn. of the pos. charge on the terminal donor in the excited state.

L17 ANSWER 18 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1996:523992 Document No. 125:167597 Preparation of naphthol derivatives as superoxide production inhibitors. Kobori, Takeo; Aida, Kenichi; Sugimoto,

Kikuo; Fujita, Mikako; Kondo, Sei; Yazawa, Kazuyoshi; Masuzawa, Yasuo; Kano, Mayumi (Sagami Chem Res, Japan). Jpn. Kokai Tokkyo Koho JP 08151341

A2 19960611 Heisei, 15 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 95-172577 19950707. PRIORITY: JP 94-229117 19940926.

GI For diagram(s), see printed CA Issue.

AB The title compds. I [ring A = benzene ring, thiazole ring, etc.; R1 = H, alkyl, etc.; R2 = halo, etc.; R3, R4 = H, nitro, etc.; m = 0 - 2; n = 1 - 4; a proviso is given] are prep'd. In a test using HL-60 cells, the title compd. II (prepn. given) in vitro showed IC50 of 4 .mu.g/mL against superoxide prodn.

L17 ANSWER 19 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1996:446496 Document No. 125:114485 Preparation of 1-acyl-4-[acylamino(methyl)]piperidines and analogs as substance P antagonists. Ofner, Silvio; Veenstra, Siem Jacob (Ciba-Geigy A.-G., Switz.). PCT Int. Appl. WO 9610562 A1 19960411, 69 pp. DESIGNATED STATES: W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, US, UZ, VN; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR,

GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG.  
(English). CODEN: PIXXD2. APPLICATION: WO 95-EP3681 19950919.  
PRIORITY:  
CH 94-2966 19940930.

GI



I

AB Title compds. [I; R1 = Bz, naphthoyl, cycloalkanoyl, etc.; R2 = cycloalkyl, Ph, naphthyl, etc.; R3 = (alkoxy)alkyl, dialkylaminoalkyl, alkanoyl(methyl), etc.; R4 = H, alkyl, alkanoyl(methyl), etc.; NR3R4 = heterocycle; Z = bond, CH2, CH2CH2, CO, CH(OH), etc.] were prep'd. Thus, (2R,4S)-1-[1-[3,5-bis(trifluoromethyl)benzoyl]-2-(4-chlorobenzyl)-4-piperidinyl]-3-ethylurea inhibited (sic) substance P binding at bovine retina at 7.6nM in vitro.

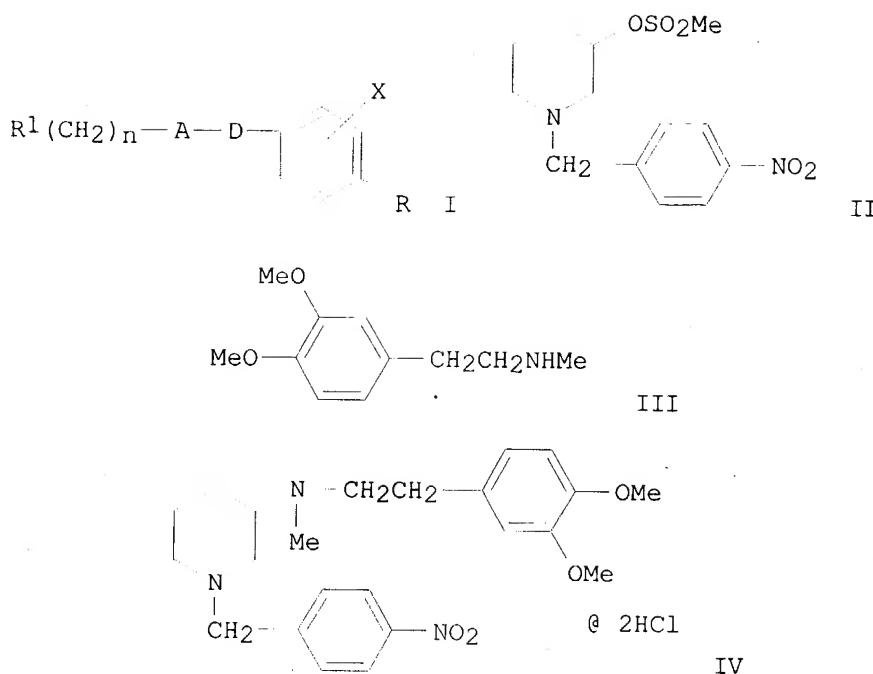
L17 ANSWER 20 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1996:393924 Document No. 125:58333 preparation of novel pyridine derivatives

as antiarrhythmic agents. Chung, You Sup; Park, Sung Dae; Kwon, Lae Sung;

Shin, Hong Sub; Tanabe, Shigeru (C and C Research Labs., S. Korea). PCT Int. Appl. WO 9605174 A1 19960222, 61 pp. DESIGNATED STATES: W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KE, KG, KZ, LK, LR, LT, LV, MD, MG, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TT, UA, US, UZ, VN; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (Japanese). CODEN: PIXXD2. APPLICATION: WO 95-JP1134 19950607.

PRIORITY: JP 94-192499 19940816.

GI



AB The title compds. [I; R = NO<sub>2</sub>, alkylsulfonamido; R<sub>1</sub> = (un)substituted Ph, quinolyl; A = 6-membered N-heterocycle residue, etc.; D = alkylene, CO, SO<sub>2</sub>, etc.; X = H, halo; n = 0-3], effective K channel blockers useful in treating arrhythmia with little side effects, are prep'd. Reaction of

mmol mesylate (R)-II with excess amine III in MeOH and acidification with HCl gave 0.85 salt IV, which at 10<sup>-6</sup> M showed an action potential duration

(APD90) ratio of 108.3 at 3 Hz and 1 Hz, vs. 37.6 with a ref. compd., in an elec. stimulation test of ventricular muscle fiber

L17 ANSWER 21 OF 94 CAPLUS COPYRIGHT 1999 ACS

1996:379812 Document No. 125:49289 Inhibitors of farnesyl-protein transferase. Fisher, Thorsten E.; Wai, John S.; Culberson, J. Christopher; Saari, Walfrid S. (Merck and Co., Inc., USA) PCT

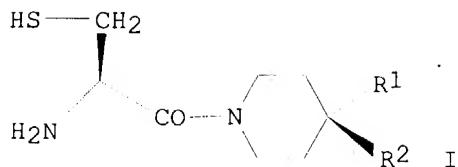
Appl.

WO 9606609 A1 19960307. 58 pp. DESIGNATED STATES: W. AM. AU. FR. BC

BR,

BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD,  
MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, US, UZ;  
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE,  
IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN:  
PIXXD2. APPLICATION: WO 95-US10827 19950825. PRIORITY: US 94-298478  
19940829.

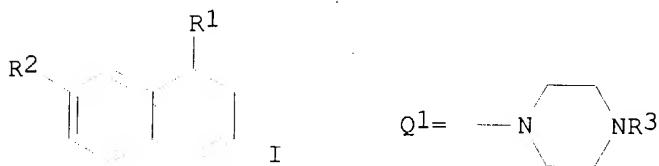
GI



AB Chemotherapeutic compns. for treatment of cancer contain substituted piperidine analogs (I; R1 = COR, CO2R, CONHR, OH, OCOR, CN, CH2OR, NHCOR, NHSO2R, etc.; R = alkyl, aryl; R2 = aryl, aralkyl, heterocycle, heteroaralkyl, etc.) as inhibitors of farnesyl-protein transferase (FTase) and farnesylation of the oncogene protein Ras.

L17 ANSWER 22 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1996:307338 Document No. 124:343334 Novel compositions containing sertraline and a 5-HT1D receptor agonist or antagonist. Chenard, Bertrand L.; Howard, Harry R.; Macor, John E.; Schulz, David W.; Sprouse, Jeffrey S. (Pfizer Inc., USA). Eur. Pat. Appl. EP 701819 A2 19960320, 51 pp.  
 DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE. (English). CODEN: EPXXDW. APPLICATION: EP 95-306249 19950907. PRIORITY: US 94-306230 19940914.

GI



AB Claimed is a pharmaceutical compn. contg. a 5-HT re-uptake inhibitor, a pharmaceutically acceptable carrier, and a compd. I [R1 = Q1, etc.; R2 = R4, etc.; R4 = H, CF3, alkyl, alkylaryl, etc.]; a proviso is given; R3 = H, alkyl, aryl, etc.]. Compds. I were assayed for 5-HT1A and 5-HT1D affinity and showed IC50 values of less than 0.6 .mu.M for at least one of said affinities. 7-Benzamido-1-(4-methyl-1-piperazinyl)naphthalene was prep'd. in several steps from 7-amino-.alpha.-tetralone.

L17 ANSWER 23 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1996:268404 Document No. 124:302259 Volume Changes Associated with Intramolecular Exciplex Formation in a Semiflexible Donor-Bridge-Acceptor Compound. Wegewijs, Bas; Verhoeven, Jan W.; Braslavsky, Silvia E. (Max-Planck-Institut fuer Strahlenchemie, Muelheim an der Ruhr, D-45413, Germany). J. Phys. Chem., 100(21), 8890-4 (English) 1996. CODEN: JPCHAX.

ISSN: 0022-3654.

AB The photophys. processes taking place in the excited state of a donor-bridge-acceptor compd. (1) in alkane solvents were studied with time-resolved laser-induced optoacoustic spectroscopy. 1 Contains an aniline/cyanonaphthalene D/A pair, sepd. by a semiflexible satd.

hydrocarbon bridge. Excitation at 308 nm leads to efficient long-range charge sepn., followed by rapid Coulomb-induced intramol. exciplex formation. By monitoring the pressure waves generated by the decay of the

excited species, three consecutive heat release processes could be discerned. In order to sep. the contributions to the obsd. acoustic signals of structural vol. changes (.DELTA.Vstr) and enthalpy changes, expts. were carried out in a series of normal alkanes, differing in their photothermal properties. A value of .DELTA.Vstr = -40 .+-. 5 mL/mol was obtained for the difference in reaction vol. between the ground state and the exciplex state of 1. This large contraction should be attributed in part to electrostriction of the solvent around the dipolar species, according to classical electrostatic theory. Furthermore, there seems to be an addnl. contraction due to the internal vol. change of 1, i.e., the conformational change involved in the intramol. exciplex formation.

L17 ANSWER 24 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1996:172220 Document No. 125:11468 Di- and tri-substituted piperidine, pyrrolidine, and hexahydro-1H-azepine non-peptide analogs promote release of growth hormone. Morriello, Gregori J.; Patchett, Arthur A.; Yang, Lihu (Merck and Co., Inc., USA). U.S. US 5492916 A 19960220, 70 pp. Cont.-in-part of U.S. Ser. No. 173,449, abandoned. (English). CODEN: USXXAM. APPLICATION: US 94-323988 19941017. PRIORITY: US 93-173449 19931223.

GI

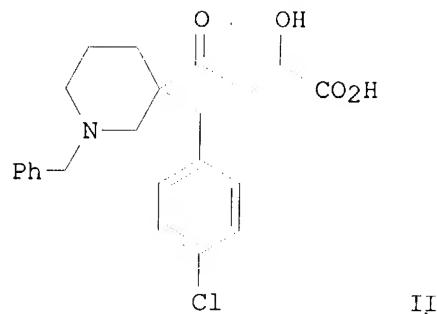
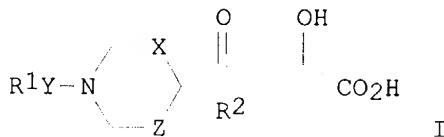
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The present invention is directed to certain novel compds. identified as di- and tri-substituted piperidines, pyrrolidines, and hexahydro-1H-azepines of the general structural formula I wherein: R1 = e.g., C1-C10 alkyl, aryl, aryl(C1-C6 alkyl); R2 = e.g., H, C1-6 alkyl, C3-7 cycloalkyl; X = e.g., H, CN, (CH2)qNR2COR2, (CH2)qNR2CO(CH2)t-aryl; Y = e.g., H, C1-10 alkyl, (CH2)t-aryl; R4 and R5 are independently, e.g., Cl-6 alkyl; A = (CH2)xCR7R7a(CH2)y or Z(CH2)xCR7R7a(CH2)y where x and y are independently 0, 1, 2, or 3; Z is NR6a or O, where R6a = H or C1-6 alkyl; R7 and R7a are independently, e.g., H, C1-6 alkyl, CF3; n is 1, 2, or 3; q is 0, 1, 2, 3, 4; t is 0, 1, 2, or 3. These compds. promote the release of growth hormone in humans and animals (no data). This property can be utilized to promote the growth of food animals to render the prodn. of edible meat products more efficient, and in humans, to treat physiol. or medical conditions characterized by a deficiency in growth hormone secretion, such as short stature in growth hormone deficient children, and to treat medical conditions which are improved by the anabolic effects of growth hormone. Growth hormone releasing compns. contg. such di- and trisubstituted piperidines, pyrrolidines, and hexahydro-1H-azepines as the active ingredient thereof are also disclosed. Thus, e.g., amide coupling of nipecotate deriv. II.HCl (prepn. given) with tryptophan amide III (prepn. given), chromatog. sepn., and deprotection afforded enantiomerically pure IV.HCl and its diastereomer at the 3-position of the nipecotate.

L17 ANSWER 25 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1996:35029 Document No. 124:232250 Piperidinyldioxobutanoic acid  
derivatives

as inhibitors of influenza endonuclease. Selnick, Harold G.; Ponticello, Gerald S.; Baldwin, John J.; Tomassini, Joanne E. (Merck and Co., Inc., USA). U.S. US 5475109 A 19951212, 16 pp. (English). CODEN: USXXAM.  
APPLICATION: US 94-324190 19941017.

GI



AB Dioxobutanoic acids substituted with piperidine or similar N-substituted satd. cycloalkyls, I or pharmaceutically acceptable salt, hydrate or crystal forms thereof, wherein: X is CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>, or a bond; Z is CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>, or a bond; Y is CH<sub>2</sub>, CO, SO<sub>2</sub>, or a bond; R<sub>1</sub> and R<sub>2</sub> are independently selected from the following: branched or unbranched C<sub>1</sub>-6 alkyl, C<sub>1</sub>-6 alkyloxy, NC<sub>1</sub>-6 alkyl, C<sub>3</sub>-8 cycloalkyl, Ph, naphthyl, pyridyl,

furanyl, thienyl, or quinolinyl, any of which may be substituted once or twice with C<sub>1</sub>-5 alkyl, C<sub>3</sub>-8 cycloalkyl, Ph, quinolinyl, pyridyl, furanyl, thienyl, C<sub>1</sub>-6-alkoxy, Br, F, or Cl, are found to inhibit the cap-dependent

endonuclease of influenza virus. These compds. are useful in the prevention or treatment of infection by influenza virus and the treatment of influenza, either as compd., pharmaceutically acceptable salts, pharmaceutical compn. ingredients, whether or not in combination with other antivirals, immunomodulators, antibiotics or vaccines. Methods of treating influenza and methods of preventing or treating infection by influenza virus are also described. Thus, e.g., treatment of N-benzyl-3-acetyl-3-(4-chlorobenzyl)piperidine with di-Me oxalate and NaH followed by HCl afforded 4-[N-benzyl-3-(4-chlorobenzyl)-piperidin-3-yl]-2,4-dioxobutanoic acid hydrochloride (II.HCl) which inhibited alfalfa mosaic virus primed flu transcription with IC<sub>50</sub> = 1.1 .mu.M.

L17 ANSWER 26 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1995:951172 Document No. 124:8627 Preparation of piperidines, pyrrolidines and hexahydro-1H-azepines which promote the release of growth hormone. Morriello, Gregori J.; Patchett, Arthur A.; Yang, Lihu; Chen, Meng H.;

Nargund, Ravi (Merck and Co., Inc., USA). PCT Int. Appl. WO 9513069 A1 19950518, 417 pp. DESIGNATED STATES: W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MN, NO, NZ, PL, RO, RU, SI, SK, TJ, TT, UA, US, US, US, UZ; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 94-US12816 19941107. PRIORITY: US 93-149441 19931109; US 93-165149 19931210; US 93-173449 19931223; US 94-323994 19941017; US 94-323988 19941017; US 94-323998 19941017.

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

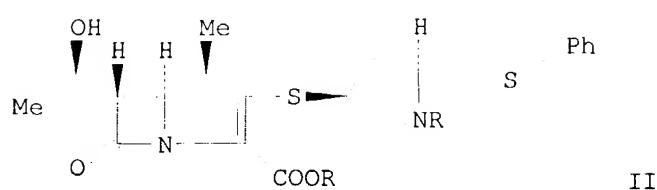
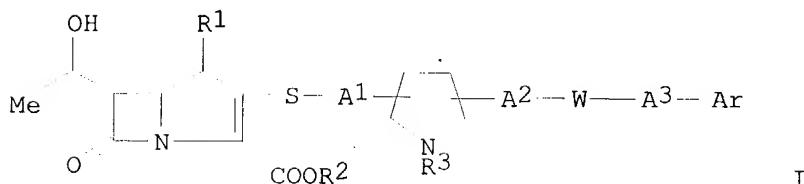
AB The title compds. [I; A = (un)substituted alkylene; R1 = (un)substituted alkyl, (un)substituted aryl, (un)substituted heteroaryl, (un)substituted Ph, (un)substituted naphthyl, etc.; R3 = H, phenylalkyl, naphthylalkyl, alkyl, cycloalkyl, halogen, etc.; R4, R5 = H, (un)substituted alkyl; W = H, CN, (un)substituted CO2H, (un)substituted CONH2, etc.; X = H, CN, (un)substituted aminoalkyl, etc; Y = H, (un)substituted alkyl, arylalkyl, etc.; n = 1-3] (e.g., II), which promote the release of growth hormone in humans and animals (no data) and can be utilized to promote the growth of food animals to render the prodn. of edible meat products more efficiently

(no data), and in humans to treat physiol. or medical conditions characterized by a deficiency in growth hormone secretion (no data), are prep'd. I-contg. growth hormone-releasing formulations are claimed.

L17 ANSWER 27 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1995:931372 Document No. 123:339535 Preparation of carbapenem derivatives as

antibacterials. Nakagawa, Susumu; Fukatsu, Hiroshi; Ushijima, Ryosuke (Banyu Pharmaceutical Co., Ltd., Japan). PCT Int. Appl. WO 9523150 A1 19950831, 256 pp. DESIGNATED STATES: W: AU, CA, JP, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (Japanese). CODEN: PIXXD2. APPLICATION: WO 95-JP280 19950224. PRIORITY: JP 94-52686 19940225; JP 94-64606 19940328; JP 94-107568 19940422; JP 94-110289 19940426; JP 94-114288 19940428.

GI



AB The title compds. [I; R1 represents hydrogen or lower alkyl; R2 represents

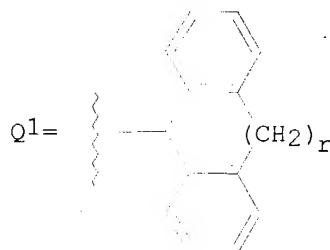
hydrogen or a neg. charge; R3 represents hydrogen or lower alkyl; Ar represents lower alkyl, lower alkylsulfamoyl, etc. (each of which may be substituted by hydroxyl, di(lower alkyl)sulfonyl, etc.), or Ph, naphthyl or a group of formula .alpha. or .beta. (each of which may be substituted by hydroxyl, di(lower alkyl)sulfonyl, etc.), wherein A4 and A5 represent each a single bond, -NHSO2-, etc., and Het represents pyrrolinyl, 1,4-diazabicyclo[2.2.2]octyl, etc. (each of which may be substituted by hydroxyl, carbamoylated lower alkyl, etc.); A1, A2, and A3 represent each a single bond or lower alkylene which may be substituted by lower alkyl, lower alkylsulfamoyl, etc. (each of which may be substituted by hydroxyl, di(lower alkyl)sulfonyl, etc.) or may be substituted by pyridyl, pyridino, etc. (each of which may be substituted by lower alkyl, carbamoylated lower alkyl, etc.); and W represents sulfur, a single bond, etc.] and their pharmaceutically acceptable salts are prep'd. Thus, a soln. of p-nitrophenyl (1R,5S,6S)-2-diphenoxypyrophosphoryloxy-6-[(1R)-1-hydroxyethyl]-1-methyl-1-carbapen-2-em-3-carboxylate and (3S,5S)-3-mercaptop-1-p-nitrobenzyloxycarbonyl-5-(phenylthiomethyl)-pyrrolidine (prepn. given) in MeCN contg. diisopropylamide was allowed to react at 50.degree. overnight to give 60% the title compd. II (R = p-nitrobenzyloxycarbonyl), which was deprotected to give the monosodium salt of II [R = H]. In an in vitro study, this had an IC50 of 0.39 .mu.g/mL against *Staphylococcus aureus*.

L17 ANSWER 28 OF 94 CAPLUS COPYRIGHT 1999 ACS

1995:896131 Document No. 123:314523 Preparation of aspartic acid derivatives

and homologs thereof for treatment of neurological diseases.. Carrera, Jesus Ezquerro; Esteban, Almudena Rubio; Mann, Andre; Schoenfelder, Angele; Schoepp, Darryle Darwin; Tercero, Conception Pedregal; Wermuth, Camille-Georges (Universite Louis Pasteur, Fr.; Lilly S.A.; Lilly, Eli, and Co.). Eur. Pat. Appl. EP 656345 A1 19950607, 24 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE. (English). CODEN: EPXXDW. APPLICATION: EP 94-308952 19941202. PRIORITY: GB 93-24872 19931203.

GI



AB Z(CH<sub>2</sub>)<sub>q</sub>Y(CH<sub>2</sub>)<sub>n</sub>CHX(CH<sub>2</sub>)<sub>m</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H [m = 0-2; n, q = 0-5; p = 0, 1; X = CO<sub>2</sub>H, tetrazolyl; Y = CH:CH; Z = (substituted) Ph, naphthyl, thieryl, CHR1R2, :CR1R2, Q1; R1, R2 = (substituted) Ph, naphthyl, thieryl; r = 0-3; provided that when Z = Ph and m = 1, then p = 1], were prep'd. as ligands for metabotropic glutamate receptors and blockers of metabotropic glutamate receptor second messenger responses. (2R, 4R,S)-2-amino-4-(3-phenyl-2-propenyl)-1,5-pentanedioic acid was prep'd. in several steps from (4R)-1,1-dimethylethyl-4-(3-ethoxy-3-oxopropenyl)-2,2-dimethyl-3-oxazolidinecarboxylate. Preferred I showed IC50 <100 .mu.m for selective displacement of (1S,3R)-ACPD in rat brain membranes.

L17 ANSWER 29 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1995:814593 Document No. 123:240722 Picosecond time-dependent Stokes shift studies of fluoroprobe in liquid solution. Middelhoek, E. R.; van der Meulen, P.; Verhoeven, J. W.; Glasbeek, M. (Laboratory for Physical Chemistry, University of Amsterdam, Nieuwe Achtergracht 127, WS Amsterdam, 1018, Neth.). Chem. Phys., 198(3), 373-80 (English) 1995. CODEN: CMPHC2.

ISSN: 0301-0104.

AB We report on a picosecond spectroscopic study of the dynamical Stokes shift of fluoroprobe in the lowest excited state in the solvents diethylether and ethylacetate. Time-resolved emission spectra with a time-resoln. of approx. 10 ps are presented. The spectra reflect dynamical Stokes shifts of a few thousand wave nos. within 10-100 ps after the pulsed laser excitation. The time-dependent shifts are representative of the solvation dynamics of fluoroprobe in diethylether and ethylacetate.

L17 ANSWER 30 OF 94 CAPLUS COPYRIGHT 1999 ACS

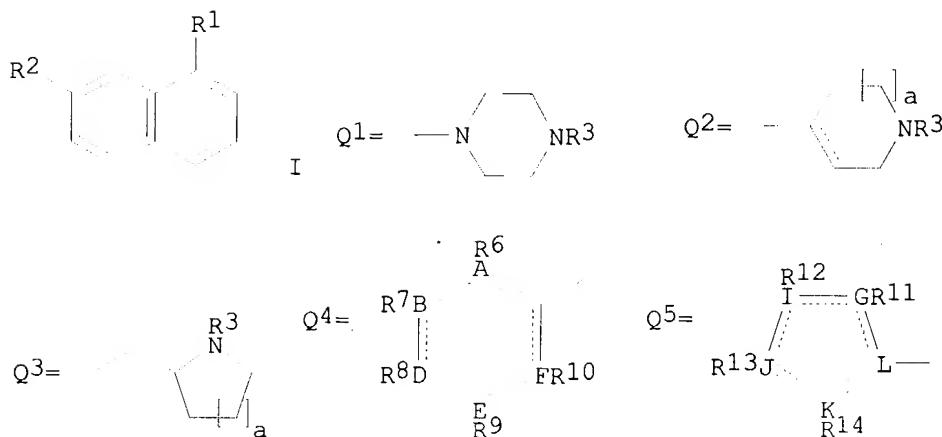
1995:776761 Document No. 124:9413 Tripeptides as selective inhibitors of src-SH2 phosphoprotein interactions. Rodriguez, Marc; Crosby, Renae; Alligood, Krystal; Gilmer, Tona; Berman, Judd (Glaxo Wellcome Res. Inst., Triangle Park, NC, 27709, USA). Lett. Pept. Sci., 2(1), 1-6 (English) 1995. CODEN: LPSCM. ISSN: 0929-5666.

AB The synthesis of phosphorylated peptides Ac-Tyr(PO3H2)-Glu-D-NHCHRCH2CH2CONH2 (I; R = CH2CH2Ph, Bu, 1-naphthylmethyl, 2-naphthylmethyl) as protein tyrosine kinase inhibitors is described. Peptides I displayed activities in the micromolar range in inhibiting src-SH2 domain/epidermal growth factor receptor interactions.

L17 ANSWER 31 OF 94 CAPLUS COPYRIGHT 1999 ACS

1995:580492 Document No. 122:314570 Preparation of heterocycllynaphthalene derivatives as serotonin 5-HT1 agonists and antagonists.. Chenard, Bertrand L.; Macor, John E.; Segelstein, Barbara E. (Pfizer Inc., USA). PCT Int. Appl. WO 9421619 A1 19940929, 85 pp. DESIGNATED STATES: W: AU, BR, CA, CN, CZ, JP, KR, NO, NZ, PL, RU, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 94-US1206 19940215. PRIORITY: US 93-32042 19930316.

GI



AB      Title compds. [I; R1 = Q1-Q3, etc.; R2 = R4, OR4, OS(O)2R4, NR4R5, R4(CH2)bNH(C:X)(CH2)c, R4(CH2)bO(C:O)NH(CH2)c(C:O)NH, R4(C:O)NH(C:O)NH, (CH2)bNH(C:X)(CH2)bO(C:O)(CH2)cR4, NH(C:X)NHR4, R4O(C:O)O, O(C:O)NHR4, R4O(C:O)NH, (CH2)b(C:O)(CH2)cR4, NHS(O)2R4, C(OH)R4R5, CH(OH)R4, (C:O)NR4R5, CN, NO2, substituted alkyl, (substituted) alkenyl, alkynyl;

R3      = H, alkyl, alkylaryl, aryl; R4, R5 = Q4, Q5, H, CF3, alkyl, alkylaryl, etc.; R6-R14 = H, halo, CF3, CN, NO2, aryl, alkylaryl, alkyl, alkenyl, alkynyl, OR20, COR20, NR20R21, etc.; adjacent pairs of R6-R14 = atoms to form 5-7 membered rings; R20, R21 = H, alkyl, aryl, alkylaryl; R20R21 = atoms to form 4-7 membered rings; A, B, D, E, F, L = C, N; G, I, J, K = C, N, O, S, C:O; X = O, S; a = 0-2; b, c = 0-6; dotted line = optional double

bond; with provisos], were prep'd. These compds. are useful psychotherapeutics and are potent serotonin (5-HT1) agonists and antagonists and may be used in the treatment of depression, anxiety, eating disorders, obesity, drug abuse, cluster headache, migraine, pain and chronic paroxysmal hemicrania and headache assoc'd. with vascular disorders, and other disorders arising from deficient serotonergic neurotransmission. The compds. can also be used as centrally acting antihypertensives and vasodilators. Thus, 7-amino-.alpha.-tetralone was stirred with PhCOCl/Et3N in THF to give 85% 7-benzamido-.alpha.-tetralone.

This in THF at -78.degree. was treated with N-methylpiperazine and TiCl4 to give 83%

7-benzamido-1-(4-methyl-1-piperazinyl)-3,4-dihydronaphthalene.

The latter was refluxed with Pd/C in xylene to give title compd.

7-benzamido-1-(4-methyl-1-piperazinyl)naphthalene and 7-benzamido-1-(4-methyl-1-piperazinyl)-1,2,3,4-tetrahydronaphthalene. I showed IC50 <0.60 nM for 5-HT1A and/or 5-HT1D affinity.

L17 ANSWER 32 OF 94 CAPLUS COPYRIGHT 1999 ACS

1995:352125 Document No. 123:169535 Studies on New Acidic Azoles as Glucose-Lowering Agents in Obese, Diabetic db/db Mice. Kees, Kenneth L.; Caggiano, Thomas J.; Steiner, Kurt E.; Fitzgerald, John J., Jr.; Kates, Michael J.; Christos, Thomas E.; Kulishoff, John M.; Moore, Robin D.; McCaleb, Michael L. (Wyeth-Ayerst Research, Princeton, NJ, 08543-8000, USA). J. Med. Chem., 38(4), 617-28 (English) 1995. CODEN: JMCMAR.

ISSN:

0022-2623. OTHER SOURCES: CJACS.

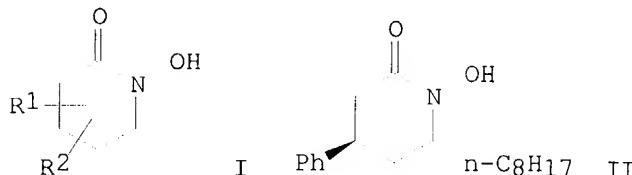
AB Bioisosteric substitution was used as a tool to generate several new structural alternatives to the thiazolidine-2,4-dione and tetrazole heterocycles as potential antidiabetic agents. Among the initial leads that emerged from this strategy, a family of acidic azoles, isoxazol-3- and -5-ones and a pyrazol-3-one, showed significant plasma glucose-lowering activity (17-42% redn.) in genetically obese, diabetic db/db mice at a dose of 100 mg/kg/day .times.4. Structure-activity relationship studies detd. that 5-alkyl-4-(arylmethyl)pyrazol-3-ones, which exist in soln. as arom. enol/iminol tautomers, were the most promising new class of potential antidiabetic agent (32-45% redn. at 20 mg/kg/d .times.4). Included in this work are convenient syntheses for several types of acidic azoles that may find use as new acidic bioisosteres in medicinal chem. such as the antidiabetic lead 5-(trifluoromethyl)pyrazol-3-one, hydroxy tautomer, and aza homologs of the pyrazolones, 1,2,3-triazol-5-ones (hydroxy tautomer) and 1,2,3,4-tetrazol-5-one heterocycles. Log P and pKa data for 15 potential acidic bioisosteres, all appended to a 2-naphthalenylmethyl residue so as to maintain a similar distance between the acidic hydrogen and arene nucleus, are presented. This new data set allows comparison of a wide variety of potential acid mimetics (pKa 3.78-10.66; log P -0.21 to 2.76) for future drug design.

L17 ANSWER 33 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1994:508528 Document No. 121:108528 1-Hydroxy-2-piperidinone antiinflammatory agents. Honn, Kenneth V.; Johnson, Carl R.; Chen, Yungfa; Shimoji, Katsuichi; Marnett, Lawrence J. (Biomide Investment Ltd. Partnership, USA; Vanderbilt Univ.). U.S. US 5292884 A 19940308, 16 pp. Cont.-in-part of U.S. 5,234,933. (English). CODEN: USXXAM.

APPLICATION:

US 92-959999 19921013. PRIORITY: US 91-785927 19911031.

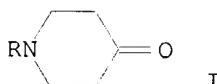
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AB The title compds. I (R1 = C1-24 alkyl; R2 = PhCH2), which are 5-lipoxygenase (no data) and 12-lipoxygenase inhibitors, useful as antiinflammatory agents, are prep'd., and I-contg. formulations presented. Thus, hydroxypiperidinone II, prep'd. from 3-hydroxy-5-phenyl-1,3-cyclohexanedione in 6 steps, demonstrated IC50 against 12-lipoxygenase of 0.15 .mu.M.

L17 ANSWER 34 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1994:323213 Document No. 120:323213 Synthesis and exploratory photophysical investigation of donor-bridge-acceptor systems derived from N-substituted 4-piperidones. Scherer, T.; Hielkema, W.; Krijnen, B.; Hermant, R. M.; Eijckelhoff, C.; Kerkhof, F.; Ng, A. K. F.; Verleg, R.; van der Tol, E. B.; et al. (Lab. Org. Chem., Univ. Amsterdam, Amsterdam, 1018 WS, Neth.). Recl. Trav. Chim. Pays-Bas, 112(10), 535-48 (English) 1993. CODEN: RTCPA3. ISSN: 0165-0513. OTHER SOURCES: CASREACT 120:323213.

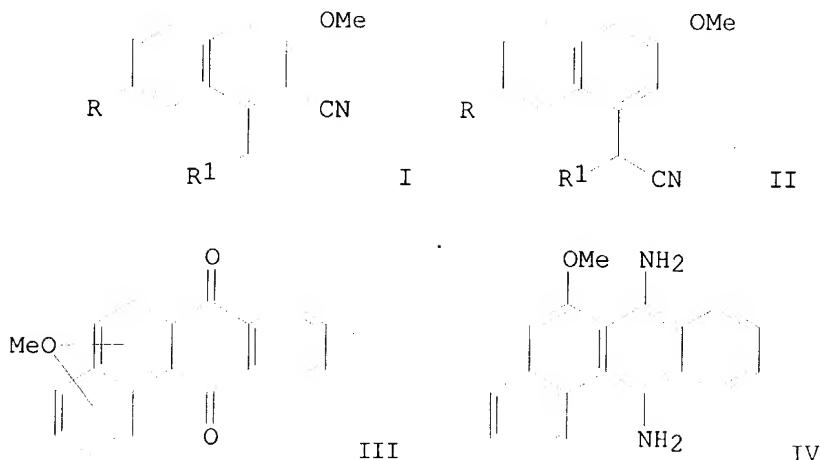
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AB A two-step synthesis for N-aryl- and N-alkyl-substituted 4-piperidones I [R = Ph, 4-MeOC<sub>6</sub>H<sub>4</sub>, 4-MeC<sub>6</sub>H<sub>4</sub>, 3,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 4-FC<sub>6</sub>H<sub>4</sub>, 4-PhC<sub>6</sub>H<sub>4</sub>, 2,4,6-Me<sub>3</sub>C<sub>6</sub>H<sub>2</sub>, 4-Me(CH<sub>2</sub>)<sub>5</sub>C<sub>6</sub>H<sub>4</sub>, 4-Me(CH<sub>2</sub>)<sub>13</sub>C<sub>6</sub>H<sub>4</sub>, cyclohexyl, 4-BrC<sub>6</sub>H<sub>4</sub>, 4-ClC<sub>6</sub>H<sub>4</sub>, 1-phenyl-4-piperidyl] is reported in which the N substituent can easily be varied. A no. of intramol. donor-acceptor systems was synthesized from these piperidones by conversion of the carbonyl functionality. The influence of the N-aryl donor on the electronic absorption and fluorescence spectra was investigated systematically. It was concluded that some systems can be used as efficient fluorescent probes with a high sensitivity for solvent polarity.

L17 ANSWER 35 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1994:269790 Document No. 120:269790 LDA (lithium diisopropylamide) mediated reactions of 1-naphthalynes with lithiated acetonitriles and 1,4-dipolar nucleophilic anions. Biehl, Edward R.; Deshmukh, A. Rakeeb; Dutt, Mahesh (Dep. Chem., South. Methodist Univ., Dallas, TX, 75275, USA). *Synthesis* (9), 885-8 (English) 1993. CODEN: SYNTBF. ISSN: 0039-7881. OTHER SOURCES: CASREACT 120:269790.

GI



AB 3-Bromo-2-methoxy- (5) and 3-bromo-2-methoxy-6-methylnaphthalene (6) yield

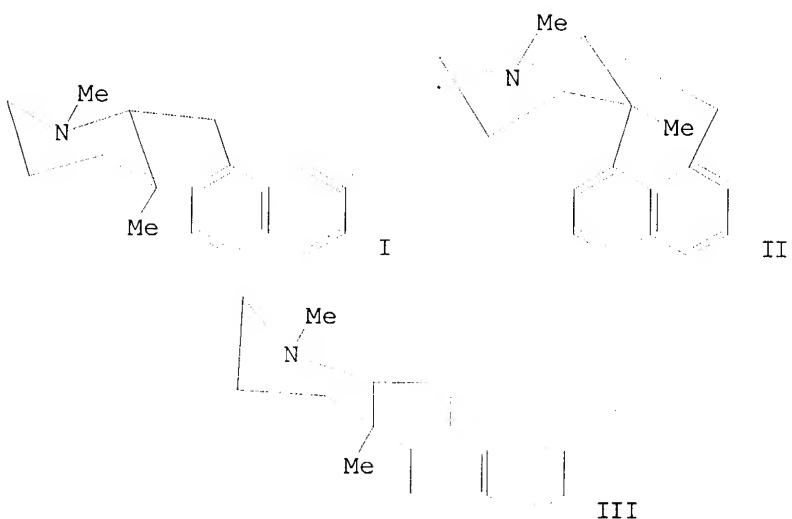
1-naphthalyne intermediates which react with  $\alpha$ -lithiated nitriles  $R_1CH(Li)CN$  [ $R_1 = 4$ -MeOC<sub>6</sub>H<sub>4</sub>, 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 2-, 3-thienyl, 2-, 3-pyridyl, 2-benzimidoyl] to give both rearranged naphthalene-2-carbonitriles I and  $\alpha$ -naphthylated acetonitriles II ( $R = H, Me$ ). Product distributions favoring rearranged nitriles I were obtained from LDA-mediated reactions of 5 with arylacetonitriles and thiopheneacetonitriles. Similar treatment

I, of 6 gave product distributions heavily in favor of rearranged nitriles presumably due to the ability of the addnl. 7-Me group to increase the rate of cyclization of the initial aryne-nitrile anion adduct, the crucial

step in the rearrangement pathway. However, treating 5 or 6 with  $\alpha$ -lithiated pyridylacetonitriles or 2-benzimidazolylacetonitrile gave product distributions heavily in favor of  $\alpha$ -naphthylated acetonitriles II. Several precursors to methoxy-substituted 1-naphthalynes undergo cycloaddn. with the dipolar nucleophilic precursors

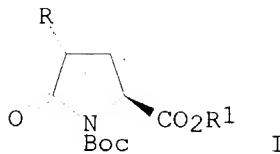
3-cyanophthalide to give benz[a]anthracenediones III (MeO attached at 3-, 5- or 6-position) and with  $\alpha$ -cyano-o-tolunitrile to give benz[a]anthracenediamine IV.

L17 ANSWER 36 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1994:163951 Document No. 120:163951 Intramolecular alkylations of aromatic  
compounds. XXX. Synthesis of cis-A-8,11a-dimethyl-7a,8,9,10,11,11a-  
hexahydro-7H-naphtho[1,8-fg]quinoline and cis-B-6b,10-dimethyl-  
6b,7,8,9,10,10a-hexahydro-11H-naphtho[2,1-g]-1-pyrindine. Reinmann,  
Eberhard; Poeschl, Klaus; Lotter, Hermann (Inst. Pharm.  
Lebensmittelchem.,  
Univ. Muenchen, Munich, D-80333, Germany). Arch. Pharm. (Weinheim,  
Ger.), 326(11), 917-19 (German) 1993. CODEN: ARPMAZ. ISSN: 0365-6233.  
GI



AB The stereoselective cyclization of 1,3-dimethyl-2-(1-naphthylmethyl)-1,2,5,6-tetrahydropyridine (I) proceeded under mild conditions to give the title compds. II and III.

L17 ANSWER 37 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1994:135094 Document No. 120:135094 Stereoselective reactions of lithium enolates derived from N-BOC protected pyroglutamic esters. Ezquerro, Jesus; Pedregal, Concepcion; Rubio, Almudena; Yruretagoyena, Belen; Escribano, Ana; Sanchez-Ferrando, Francisco (Cent. Invest. Lilly, S. A., Valdeolmos, 28130, Spain). Tetrahedron, 49(38), 8665-78 (English) 1993. CODEN: TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT 120:135094.



AB The lithium enolates of protected pyroglutamate esters I ( $R = H$ ,  $R1 = Et$ ,  $CMe3$ ;  $Boc = Me_3CO_2C$ ) react with electrophiles in good yield without epimerization of the chiral center. With benzyl bromides the process is stereospecific, yielding exclusively trans isomers I ( $R = PhCH_2$ ,  $4\text{-MeC}_6\text{H}_4\text{CH}_2$ ,  $4\text{-CF}_3\text{C}_6\text{H}_4\text{CH}_2$ ,  $4\text{-BrC}_6\text{H}_4\text{CH}_2$ ,  $4\text{-NCC}_6\text{H}_4\text{CH}_2$ , 2-naphthylmethyl). However, with other reactive electrophiles a 2:1 trans/cis diastereomeric mixt. was obtained, regardless of the steric bulk of the ester group.

L17 ANSWER 38 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1994:8151 Document No. 120:8151 Exciplex formation in jet-cooled donor-bridge-acceptor compounds incorporating bridges with three degrees of flexibility. Wegewijs, B.; Scherer, T.; Rettschnick, R. P. H.; Verhoeven, J. W. (Laboratory of Organic Chemistry and Laboratory of Physical Chemistry, University of Amsterdam, Nieuwe Achtergracht 129 and 127, WS Amsterdam, 1018, Neth.). Chem. Phys., 176(2-3), 349-57 (English) 1993. CODEN: CMPHC2. ISSN: 0301-0104.

AB Intramol. exciplex formation was studied in three types of donor-bridge-acceptor systems under jet-cooled conditions. While each of these contains the same aniline/cyanonaphthalene D/A pair the satd. hydrocarbon bridges differ in flexibility and length. With a flexible trimethylene bridge at least three conformers are present in the jet, which display different mechanisms of exciplex formation. The main conformer, probably fully extended, required an excess excitation energy  $\Delta E \geq 1100 \text{ cm}^{-1}$  for exciplex formation. This is thought to correspond with a mechanism in which IVR is the primary process bringing

D and A in closer proximity. A broad long-wavelength excitation is furthermore assigned to the presence of a fully folded conformer undergoing direct excitation into the exciplex state. In addn. a partly folded conformer appears to be present from which exciplex formation can occur at negligible excess energy. It is argued that in this partly folded conformer D and A are within harpooning range even for  $\Delta E = 0$ , implying that after excitation at the spectral origin of the acceptor chromophore electron transfer can occur followed by electrostatically driven folding to form the emissive exciplex. With two more rigid types of bridges a harpooning mechanism is also involved in formation of the exciplex. With these bridges however, the ground-state donor-acceptor distance is much better defined and is furthermore too large to allow electron transfer at  $\Delta E = 0$ . As a result exciplex formation sets in

only at excess energies sufficiently high to extend the harpooning range to or beyond the actual ground-state distance.

L17 ANSWER 39 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1994:8088 Document No. 120:8088 Formation of extended and folded charge separated states of donor-spacer-acceptor molecules with flexible and semirigid  $\sigma$ -bond spacers. Schuddeboom, Wouter; Scherer, Taco; Warman, John M.; Verhoeven, Jan W. (IRI, Delft Univ. Technol., Delft, 2629 Neth.). J. Phys. Chem., 97(50), 13092-8 (English) 1993. CODEN: JPCHAX. ISSN: 0022-3654. OTHER SOURCES: CJACS.

AB Charge sepn. resulting from photoexcitation of donor-spacer-acceptor mols., D(S)A, with an anilino (An) donor, a naphthalene (N) or cyanonaphthalene (NCN) acceptor, and either flexible (trimethylene) or semirigid (piperidine) four .sigma.-bond spacers, has been investigated by

time resolved microwave cond. and fluorescence techniques. For the An/N pair in cyclohexane, close approach of the donor and acceptor moieties is necessary for charge sepn. For the larger driving force An/NCN couple, charge sepn. can occur in the fully extended configuration. In benzene, charge sepn. occurs in the extended configuration for both D/A pairs.

For the trimethylene spacer mols., contact exciplexes are rapidly formed either by prior folding or by harpooning. For the semirigid spacer, electrostatically-driven folding, involving inversion of the piperidine ring, can occur subsequent to long-distance charge sepn. on a time scale of several nanoseconds.

L17 ANSWER 40 OF 94 CAPLUS COPYRIGHT 1999 ACS

1993:670479 Document No. 119:270479 Straight, bent and twisted intramolecular charge separated states as seen by time-resolved microwave conductivity (TRMC). Warman, John M.; Jonker, Stephan A.; Schuddeboom, Wouter; de Haas, Matthijs P.; Paddon-Row, Michael N.; Verhoeven, Jan W.; Zachariasse, Klaas A. (IRI, Delft Univ. Technol., Delft, 2629 JB, Neth.). Pure Appl. Chem., 65(8), 1723-8 (English) 1993. CODEN: PACHAS. ISSN: 0033-4545.

AB The application of the TRMC technique to the study of non Franck-Condon charge sepd. states formed subsequent to vertical photoexcitation is illustrated with examples which include long-distance intramol. electron transfer and mol. folding or twisting.

L17 ANSWER 41 OF 94 CAPLUS COPYRIGHT 1999 ACS

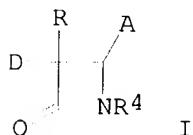
1993:517027 Document No. 119:117027 Substituted beta-lactam compounds useful

as hypocholesterolemic agents and processes for their preparation. Burnett, Duane A.; Clader, John W.; Thiruvengadam, Tiruvettipuram K.; Tann, Chou Hong; Lee, Junning; McAllister, Timothy; Colon, Cesar; Barton, Derek H. R.; Breslow, Ronald; et al. (Schering Corp., USA). Eur. Pat. Appl. EP 524595 A1 19930127, 98 pp. DESIGNATED STATES: R: PT. (English). CODEN: EPXXDW. APPLICATION: EP 92-112425 19920721.

PRIORITY:

US 91-734652 19910723; US 91-734426 19910723.

GI



AB Title compds. I (A = BCH:CH, BC.tplbond.C, BX(CH2)p wherein B = (substituted) Ph; X = bond, NH, S(O)p, (substituted) heteroaryl, (substituted) benzofused heteroaryl, (substituted) piperazinyl(alkyl), etc., p = 0-2; R = H, F, C1-15 alkyl, C1-15 alkenyl, C1-15 alkynyl, B(CH2)h wherein h = 0-3, etc.; D = B'(CH2)mCO, B'(CH2)q, B'(C2-6 alkenylene, etc. wherein B' = naphthyl, (substituted) Ph, m = 1-5, q = 2-6; R4 = substituted Ph, heterocyclyl) or a salt thereof, are prep'd. (Me2CH)2NLi was added to Et 5-phenylvalerate in THF, followed by 4-methoxybenzylideneanisidine in CH2Cl2 to give the title (.+-.)-I (A =

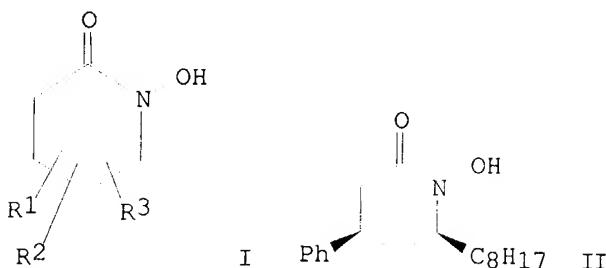
= 4-(MeO)C<sub>6</sub>H<sub>4</sub>, R = H, D = PhCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>) (II). In hyperlipidemic hamsters, II at 50 mg/kg showed a redn. of serum cholesterol and cholesterol esters of 45 and 95%, resp. Capsule and tablet formulations comprising I are given.

L17 ANSWER 42 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1993:516557 Document No. 119:116557 Long-range, photoinduced charge separation in solvent-free donor-bridge-acceptor molecules. Jortner, Joshua; Bixon, M.; Wegewijs, Bas; Verhoeven, Jan W.; Rettschnick, Rudolf P. H. (School of Chemistry, Tel Aviv University, Ramat Aviv, Tel Aviv, 69978, Israel). Chem. Phys. Lett., 205(4-5), 451-5 (English) 1993. CODEN: CHPLBC. ISSN: 0009-2614.

AB Charge sepn. in isolated supermols., consisting of an aniline or 4-methoxyaniline donor and a cyanonaphthalene acceptor connected by a semirigid bridge, is described in terms of irreversible sequential intramol. relaxation involving electron transfer from an electronically excited mol. state and electrostatically driven folding. Sequential folding of the charge transfer state extends the energy range of this state, which is accessible by radiationless electron transfer. The anal. of the intramol. electron transfer dynamics led to agreement between the distance scale for charge sepn. inferred from energetic and structural data and accounted for the excess energy dependence of the nuclear Franck-Condon vibrational overlap factors.

L17 ANSWER 43 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1993:495349 Document No. 119:95349 Cyclic hydroxamic acids and their use as lipoxygenase inhibitors.. Honn, Kenneth V.; Johnson, Carl R.; Chen, Yung Fa; Chimoji, Katsuichi; Marnett, Lawrence J. (Wayne State University, USA; Vanderbilt University). PCT Int. Appl. WO 9308803 A1 19930513, 49 pp. DESIGNATED STATES: W: JP; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE. (English). CODEN: PIXXD2. APPLICATION: WO 92-US8916 19921016. PRIORITY: US 91-785927 19911031.

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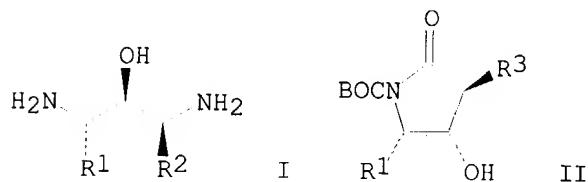


AB The title compds., i.e. 1-hydroxy-2-piperidinones I (R = alkyl, alkenyl, aryl, arylalkyl, etc.) and their use as 12-lipoxygenase antagonists are claimed. 12-Lipoxygenase antagonizes leukotriene B<sub>4</sub> and enhances the activity of 5-lipoxygenase. Are potential inflammation inhibitors, agents for the treatment of immune diseases, psoriasis, antiarteriosclerotics and treatment of ischemic heart disease or the suppression of cancer metastasis. Cyclocondensation of 5-(hydroxyimino)-3-phenyltridecanoic

acid (prepd. in several steps) gave cis-1-hydroxy-6-octyl-4-phenyl-2-pyridinone cis-I and trans-I. Cis-I inhibited the formation of arachidonic acid metabolites with an IC<sub>50</sub> of 0.6 M.

L17 ANSWER 44 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1993:448902 Document No. 119:48902 A diastereoselective synthesis of pseudo-C2-symmetric 1,3-diamino-2-propanols as core units in HIV protease inhibitors. Wittenberger, Steven J.; Baker, William R.; Donner, B. Gregory (Pharm. Prod. Div., Abbott Lab., Abbott Park, IL, 60064, USA). Tetrahedron, 49(8), 1547-56 (English) 1993. CODEN: TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT 119:48902.

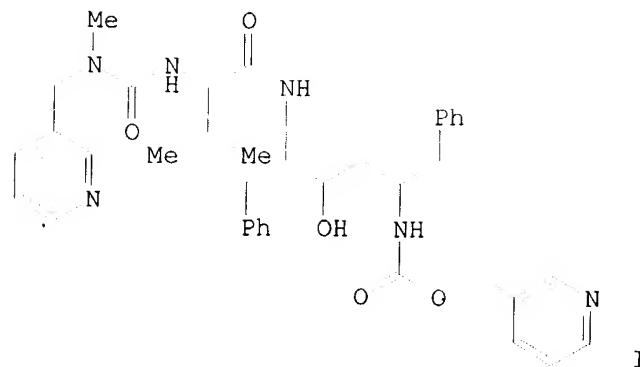
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AB Inhibitors of HIV-1 protease are effective against the proliferation of HIV-1 infection in vitro. Based on the inherent symmetry of the protease homodimer, C2-sym. and pseudo-C2-sym. inhibitors have been designed, synthesized, and demonstrated to be potent inhibitors of HIV-1 protease and effective in arresting the spread of HIV-1 in vitro. A novel synthesis of the pseudo-C2-sym. 1,3-diamino-2-propanol core unit I, the key subunit in such HIV-1 protease inhibitors is reported. Alkylation of the dianion of N-Boc hydroxylactam II (R3 = H) is highly diastereoselective and provides II (R3 = R2) in moderate to good yield. Imide ring opening, Curtius rearrangement, and deprotection lead to the desired diamino alc. core unit I. A no. of substituents, arom. and heteroarom. were included in the R1 and R2 side chains.

L17 ANSWER 45 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1993:192283 Document No. 118:192283 amino acid derivatives as HIV-1 protease inhibitors and methods for their synthesis. Kempf, Dale J.; Codacovi, Lynn M.; Norbeck, Daniel W.; Plattner, Jacob J.; Sham, Hing L.; Wittenberger, Steven J.; Zhao, Chen (Abbott Laboratories, USA). Eur. Pat. Appl. EP 486948 A2 19920527, 154 pp. DESIGNATED STATES: R: AT, BE, DE, DK, FR, GB, GR, LU, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 91-119464 19911104. PRIORITY: US 90-616170 19901120; US 91-746020 19910815; US 91-777626 19911023.

GI



AB Certain 2-alkoxy-1,4-butanediamine derivs. are claimed. Specific compds. such as

(2S,3S,5S)-2-[N-[N-methyl-N-[(2-pyridyl)methyl]amino]carbonyl]vinylaminylamino]-5-[N-[(3-pyridinyl)methoxycarbonyl]amino]-1,6-diphenyl-3-hydroxyhexane I, their salts, and prodrug forms thereof are claimed. The use of such compds. for the manuf. of pharmaceuticals for the treatment of

HIV infections and their use for the inhibition of HIV protease are claimed. I in vivo was an HIV-1 protease inhibitor and it was active against HIV-13b.

L17 ANSWER 46 OF 94 CAPLUS COPYRIGHT 1999 ACS

1993:49035 Document No. 118:49035 A dramatic effect of the donor ionization potential on the apparent barrier to intramolecular exciplex formation in jet-cooled, bichromophoric molecules. Wegewijs, B.; Ng, A. K. F.; Rettschnick, R. P. H.; Verhoeven, J. W. (Lab. Org. Chem., Univ. Amsterdam,

Nieuwe Achtergracht 129, WS Amsterdam, 1018, Neth.). Chem. Phys. Lett., 200(4), 357-63 (English) 1992. CODEN: CHPLBC. ISSN: 0009-2614.

AB The fluorescence of 3 nearly identical donor-bridge-acceptor mols. was studied under jet-cooled conditions. These compds. contain a 1-cyanonaphthalene group as an electron acceptor (A) and an anilino deriv.

as an electron donor (D). Their only difference is in the substituent on the para position of the anilino group and therefore in ionization potential (IP). D and A are interconnected by a satd. hydrocarbon bridge of limited flexibility, which holds D and A far apart in the electronic ground state. Nevertheless, an intramol. exciplex was formed upon excitation of the cyanonaphthalene group with sufficient excess vibrational energy. The barrier to this exciplex formation appears to be much lower than the barrier predicted for folding the bridge to bring D and A in close contact and also, the mol. with the lowest IP has by far the lowest barrier. This is taken as conclusive evidence that long-range electron transfer is the 1st step in the exciplex formation and dets. the height of the barrier. The subsequent folding of the bridge would then be

a result of the Coulombic attraction forces between D and A.

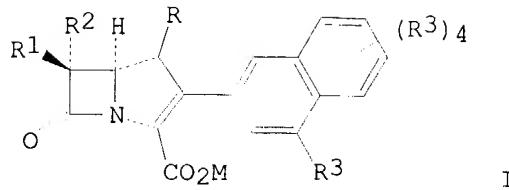
L17 ANSWER 47 OF 94 CAPLUS COPYRIGHT 1999 ACS

1992:448210 Document No. 117:48210 Preparation of 2-naphthylcarbapenems as antibacterial agents. Dininno, Frank P.; Greenlee, Mark L. (Merck and Co., Inc., USA). Eur. Pat. Appl. EP 466254 A1 19920115, 112 pp.

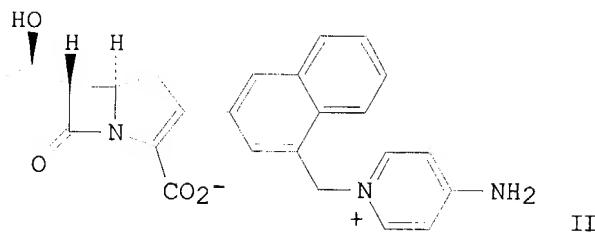
DESIGNATED STATES: R: CH, DE, FR, GB, IT, LI, NL. (English). CODEN: EPXXDW. APPLICATION: EP 91-201706 19910703. PRIORITY: US 90-551699

GI

19900711; US 90-594213 19901009.



I



II

AB Title compds. I [R = H, Me; R1, R2 = H, Me, Et, Me2CH, HOCH2, MeCH(OH), Me2C(OH), FCH2CH(OH), F2CHCH(OH), F3CCH(OH), MeCHF, MeCF2, Me2CF; each R3 = H, AX, CF3, halo, (substituted) C1-4 alkoxy, OH, (substituted) carbamoyloxy, N3, cyano, tetrazolyl, etc.; A = spacer; X = (substituted) N-contg. heterocyclyl which may be pos. charged; M = H, carboxy-protecting group, atoms to complete an ester group, alkali metal cation, neg. charge, etc.; with provisos] were prep'd. as antibacterial agents (no data). Thus, allyl (5R,6S)-2-(1-hydroxymethyl-3-naphthyl)-6-[1R-(allyloxycarbonyloxy)ethyl]carbapen-3-em-3-carboxylate (prepn. given) was tosylated and then reacted with NaI in acetone to give the iodomethylnaphthyl deriv. N-Alkylation of 4-aminopyridine by the latter, followed by deprotection gave title compd. II.

L17 ANSWER 48 OF 94 CAPLUS COPYRIGHT 1999 ACS

1992:402313 Document No. 117:2313 Interaction of flexible analogs of N-methyl-4-phenyl-1,2,3,6-tetrahydropyridine and of N-methyl-4-phenylpyridinium with highly purified monoamine oxidase A and B.

Krueger,

Matthew J.; Efange, S. M. N.; Michelson, Robert H.; Singer, Thomas P. (Dep. Biochem., Univ. California, San Francisco, CA, 94143, USA). Biochemistry, 31(24), 5611-15 (English) 1992. CODEN: BICHAW. ISSN: 0006-2960. OTHER SOURCES: CJACS.

AB Sixteen analogs of MPTP of varying degrees of flexibility were studied as substrates of highly purified MAO A and B. The relative effectiveness of the various tetrahydropyridines as substrates of MAO A and B were evaluated in terms of the function turnover no./Km, as detd. by initial rate measurements. The insertion of a methylene bridge between the Ph

and

tetrahydropyridine moieties of MPTP to yield N-methyl-4-benzyl-1,2,3,6-tetrahydropyridine, rendering the mol. more flexible, greatly enhances reactivity with MAO B, but not with MAO A, as compared with MPTP itself, in accord with data in the literature (S. K. Youngster et al., 1989a). The ethylene-bridged MPTP analog, on the other hand, is a far better substrate of both forms of MAO than is MPTP itself. The effect of mol. flexibility on the rate of oxidn. of these compds. is obscured by substituents on the arom. ring. Branching and rigidity were detrimental to the activity as substrates of both forms of MAO. Those analogs of I which contain small electron-withdrawing substituents in the Ph ring were

more selective to MAO B, whereas those substituted with bulky groups were selectively oxidized by MAO A. The substrate binding site of MAO A probably contains a lipophilic pocket larger than that found in a similar site in MAO B.

L17 ANSWER 49 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1992:128683 Document No. 116:128683 Novel piperidine, tetrahydropyridine, and pyrrolidine derivatives useful as antihypertensives, process for their preparation, and pharmaceutical compositions containing them. Lavielle, Gilbert; Laubie, Michel; Colpaert, Francis (ADIR et Cie., Fr.). Eur. Pat.

Appl. EP 466585 A1 19920115, 57 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE. (French). CODEN: EPXXDW. APPLICATION: EP 91-401915 19910710. PRIORITY: FR 90-8729 19900710. AB Title compds. R1ABR2 [I; R1 = (un)substituted 1-naphthyl or its 3,4-dihydro or 1,2,3,4-tetrahydro derivs., 3-quinolyl, 1,4-benzodioxan-5-yl; A = single or double bond, CH<sub>2</sub>, CH; B = piperidyl, pyrrolidinyl, 1,2,3,6-tetrahydropyridyl, all bound to A at a C atom and to

R2 at the N atom; R2 = H, CH<sub>2</sub>Ph, alkyl, aminoalkyl, cyanoalkyl, benzamidoalkyl; with a variety of provisos and conditions] and salts, having 5-HT1A receptor activity, were prep'd. as antihypertensives and possibly for addnl. uses. For example, lithiation of 1-bromonaphthalene and reaction with 1-methylpiperid-4-one (73%), followed by dehydration of the resulting alc. in 48% HBr (86.65%), gave 1-methyl-4-(1-naphthyl)-1,2,3,4-tetrahydropyridine HBr salt, a title compd. This was sequentially

converted to addnl. I by hydrogenation, demethylation, N-alkylation with BrCH<sub>2</sub>CN, etc. As an example using anesthetized dogs, two compds. I showed

antihypertensive activity comparable or superior to both racemic and (+)-flesinoxan. Over 30 synthetic examples, <sup>1</sup>H-NMR data for various I and intermediates, and a receptor assay are described.

L17 ANSWER 50 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1992:101623 Document No. 116:101623 Differences in substrate specificities of monoamine oxidase A from human liver and placenta. Tan, Anthony K.; Weyler, Walter; Salach, James I.; Singer, Thomas P. (Dep. Biochem. Biophys., Univ. California, San Francisco, CA, 94143, USA). Biochem. Biophys. Res. Commun., 181(3), 1084-8 (English) 1991. CODEN: BBRCA9. ISSN: 0006-291X.

AB The substrate specificities of monoamine oxidase (MAO) A isolated from human placenta and of human liver expressed in yeast have been compared in homogeneous preps. with respect to V<sub>max</sub> and K<sub>m</sub> values for natural and synthetic substrates and K<sub>i</sub> values for competitive inhibitors. MAO A from

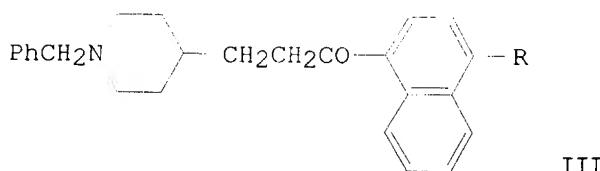
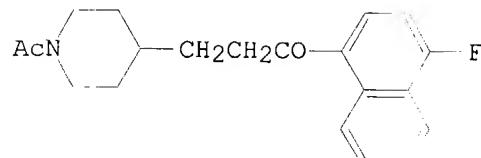
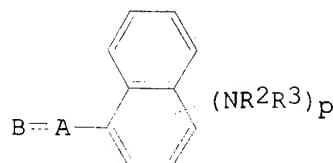
these two sources is known to differ in at least 5 amino acid residues. While the K<sub>m</sub> and K<sub>i</sub> values were nearly identical in the enzymes from these

two sources, the V<sub>max</sub> differed significantly for bulky synthetic substrates.

L17 ANSWER 51 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1992:83548 Document No. 116:83548 Preparation of piperidine derivatives containing aminonaphthyl groups as brain function improvers. Goto, Giichi; Yukimasa, Hidefumi; Ishihara, Yuji (Takeda Chemical Industries, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 03223251 A2 19911002 Heisei, 14 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 90-323493 19901126.

TRICR111. 01 09 322174 19891211.

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AB The title compds. [I; B = (substituted) satd. or unsatd. 5-7-membered aza heterocycle, e.g., piperidine, residue; A = bond, hydrocarbon residue, oxo, hydroxyimino, etc.; R2, R3 = H, (substituted) hydrocarbyl, R2R3N = heterocyclyl; p = 1, 2], useful in treating brain edema, are prep'd. Refluxing 1.0 g alkanoylnaphthalene II in concd. HCl and reaction with

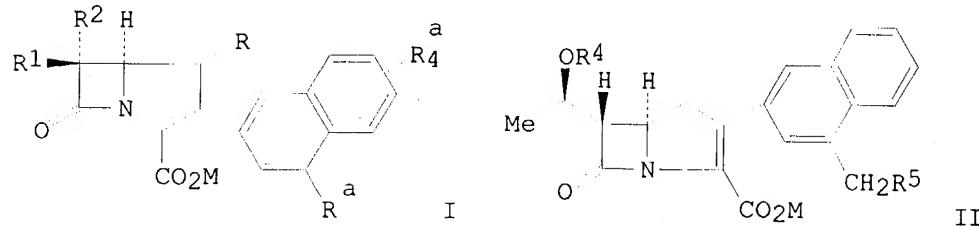
0.5

g PhCH<sub>2</sub>Br gave 0.76 g benzyl deriv. III (R = F), which (0.4 g) was heated with 50% aq. Me<sub>2</sub>NH at 70.degree. and treated with fumaric acid to give 0.46 g III (R = Me<sub>2</sub>N) fumarate (IV). IV showed acetylcholine esterase inhibition with an IC<sub>50</sub> of 4.1 .mu.M. Tablet and injection formulations were given.

L17 ANSWER 52 OF 94 CAPLUS COPYRIGHT 1999 ACS

1992:59076 Document No. 116:59076 Preparation of naphthylcarbapenems as antibiotics and antibacterials. DiNinno, Frank P.; Greenlee, Mark L. (Merck and Co., Inc., USA). U.S. US 5032587 A 19910716, 45 pp. (English). CODEN: USXXAM. APPLICATION: US 90-551699 19900711.

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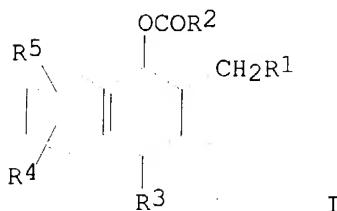
AB Title compds. [I; M = H, ester residue, cation, neg. charge, etc.; R = H, Me; R<sub>1</sub>, R<sub>2</sub> = H, Me, Et, CH<sub>2</sub>OH, MeCH(OH), etc.; 1 of Ra = [(CH<sub>2</sub>)<sub>m</sub>Q(CH<sub>2</sub>)<sub>n</sub>]pR<sub>3</sub>, etc., and the others = H, CF<sub>3</sub>, halo, OH, alkoxy, cyano, etc.; Q = bond, O, S, NH, CO, CH:CH, etc.; when p = 1, m = 0-6, and

and  $n = 1-6$ ,  $R_3 =$  pyridinium-1-yl, quinolinium-1-yl, etc.; when  $p = 1$ ,  $m = 0-6$ , and  $n = 0-6$ ,  $R_3 =$  pyridyl, quinolyl, etc.] were prep'd. as antibiotics.

and antibacterials (no data). Thus, (3*S*, 4*R*)-1-(allyloxycarbonyltriphenylphosphoranylidene)methyl-3-[(*R*)-1-

(allyloxycarbonyloxy)ethyl]-4-[(2-pyridylthio)carbonyl]methylazetidin-2-one was condensed with the Grignard reagent from 3-bromo-1-(tert-butyldimethylsilyloxyethyl)naphthalene and the deprotected product cyclized to give title compd. II (M = allyl, R4 = CH2:CH2O2C) (III; R5 = OH) which was converted in 2 steps to III (R5 = iodo). The latter was condensed with 4-aminopyridine to give, after deprotection, III (M = neg. charge, R4 = H, R5 = 4-aminopyridinium-1-yl).

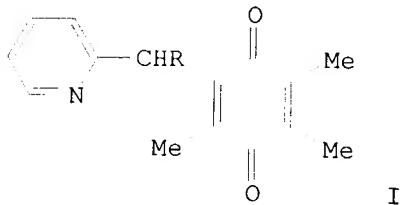
L17 ANSWER 53 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1991:471165 Document No. 115:71165 Preparation of esters of  
 2-arylmethyl-1-naphthols as 5-lipoxygenase inhibitors. Batt, Douglas G.  
 (du Pont de Nemours, E. I., and Co., USA). U.S. US 5006555 A 19910409,  
 8 pp. (English). CODEN: USXXAM. APPLICATION: US 90-466601 19900117.  
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AB Title compds. I [R1 = pyridyl, thiienyl, N-methylpyrryl, thiazolyl, methylenedioxyphenyl, (substituted) phenyl; R2 = C1-4 alkyl, C1-4 alkoxy, (CH2)nR6; n = 2-4; R3 = H, C1-4 alkyl, Br, Cl; R4, R5 = H, C1-4 alkyl, C1-4 alkoxy; R6 = H, CO2R7, NR8R8; R7, R8 = H, C1-4 alkyl], useful as antiinflammatories, were prep'd. Thus, Ac2O in pyridine was condensed with 2-phenylmethyl-1-naphthol to give 82% acetate I (R1 = Ph, R2 = Me, R3-R5 = H), which at 0.14 .mu.M gave 50% inhibition of 5-lipoxygenase and also showed 66% inhibition of arachidonic acid ear edema in mice of 100 .mu.g/ear. Formulations of I were prep'd.

L17 ANSWER 54 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1991:36117 Document No. 114:36117 Dual inhibitors of thromboxane A2 synthase and 5-lipoxygenase with scavenging activity of active oxygen species (AOS). Synthesis of a novel series of (3-pyridylmethyl)benzoquinone derivatives. Ohkawa, Shigenori; Terao, Shinji; Terashita, Zenichi; Shibouta, Yumiko; Nishikawa, Kohei (Res. Dev. Div., Takeda Chem. Ind. Ltd., Osaka, 532, Japan). J. Med. Chem., 34(1), 267-76 (English) 1991. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CJACS.

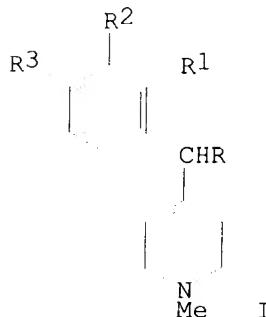
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AB A novel series of (3-pyridylmethyl)benzoquinone derivs. (e.g., I, R = e.g., alkyl, carboxyalkyl, Ph, etc.,) was synthesized for the dual purpose of inhibiting thromboxane A2 and leukotriene biosynthesis enzymes and scavenging active oxygen species (AOS). They were evaluated for inhibition of TXA2 synthase, inhibition of 5-lipoxygenase, and for their scavenging activity of AOS using the thiobarbituric acid method. 2,3,5-Trimethyl-6-(3-pyridyl-methyl)-1,4-benzoquinone (II) was the most promising deriv. since it showed efficient AOS scavenging activity (inhibition of lipid peroxidn. in rat brain homogenates: IC<sub>50</sub> = 1.8 .times. 10<sup>-6</sup>M) as well as potent, specific, and well-balanced inhibitory effects on both enzymes (inhibitory effect on TXA2 synthase in human blood, IC<sub>50</sub> = 3.3 .times. 10<sup>-7</sup>M; inhibitory effect on 5-lipoxygenase in human blood, IC<sub>50</sub> = 3.6 .times. 10<sup>-7</sup>M). In adriamycin induced-proteinuria in a rat model, compd. II at 10 mg/kg/per day (oral) suppressed proteinuria by more than 50%. The proteinuria, however, was not reduced by single administration of an inhibitor specific for thromboxane A2 synthase [(E)-7-phenyl-7-(3-pyridyl)-6-heptenoic acid] or for 5-lipoxygenase [2-(12-hydroxy-5,10-dodecadiynyl-3,5,6-trimethyl-1,4-benzoquinone)]. The proteinuria was also not reduced by administration of an AOS scavenger, 2-O-octadecylascorbic acid. Triple functional compds. such as II that specifically inhibit both enzymes as well as scavenge AOS possess a variety of pharmacol. beneficial effects.

L17 ANSWER 55 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1991:6237 Document No. 114:6237 Flexible N-methyl-4-phenyl-1,2,3,6-tetrahydropyridine analog: synthesis and monoamine oxidase catalyzed bioactivation. Efange, S. Mbera Ngale; Michelson, R. H.; Remmel, R. P.; Boudreau, R. J.; Dutta, A. K.; Freshler, A. (Dep. Radiol. Med. Chem., Univ. Minnesota, Minneapolis, MN, 55455, USA). J. Med. Chem., 33(12), 3133-8 (English) 1990. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 114:6237; CJACS.

GI



AB Eighteen analogs, e.g., I (R = H, Me; R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> = H, Me, OMe) of N-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP) were synthesized and evaluated as substrates of monoamine oxidase. In general, the flexible analogs, characterized by the presence of a methylene (or ethylene) bridge between the aryl/heteroaryl and tetrahydropyridyl moieties, were better substrates of the enzyme than the conformationally restricted MPTP. It is suggested that the increased oxidative activity of these flexible analogs reflects enhanced binding due to the ability of the aryl/heteroaryl

substituent to gain access to a hydrophobic pocket within the substrate binding site.

L17 ANSWER 56 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1990:531961 Document No. 113:131961 Substitution reactions involving organoaluminum compounds. Reaction of metalated picoline with aryl halides catalyzed by nickel and palladium complexes. Kresteleva, I. V.; Spivak, A. Yu.; Tolstikov, G. A. (Inst. Khim., Ufa, USSR). Metalloorg. Khim., 3(3), 692-6 (Russian) 1990. CODEN: MEKHEX.  
AB A direct and regioselective synthesis of 2- and 4-(arylmethyl)pyridines was carried out via reaction of Al and Zn derivs. of 2- and 4-picolines with aryl halides in the presence of Ni(PPh<sub>3</sub>)<sub>4</sub>.

L17 ANSWER 57 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1990:468160 Document No. 113:68160 Exciplex-type emission from folded and extended conformations of a donor-acceptor molecule with limited flexibility. Wegewijs, B.; Hermant, R. M.; Verhoeven, J. W.; De Haas, M. P.; Warman, J. M. (Lab. Org. Chem., Univ. Amsterdam, Amsterdam, 1018 WS, Neth.). Chem. Phys. Lett., 168(2), 185-90 (English) 1990. CODEN: CHPLBC.

ISSN: 0009-2614.  
AB The fluorescent behavior of a donor-bridge-acceptor compd. was studied in apolar solvents as a function of temp. In the ground-state conformation donor and acceptor are held far apart by the interconnecting satd. hydrocarbon bridge. Photoexcitation at room temp. in an apolar solvent nevertheless leads to exciplex-like emission at 454 nm from a folded conformation. Emission spectra at low temps. reveal a totally different fluorescence band at 380 nm that is ascribed to a charge-transfer state with a stretched conformation. With time-resolved fluorescence measurements it was shown that this state is the precursor to the folded exciplex-state, indicating that charge sepn. takes place in an extended conformation. At room temp. charge sepn. is followed by rapid Coulomb-induced interconversion to a folded conformation, thereby efficiently quenching the 380 nm fluorescence. Further confirmation of this interpretation was obtained by time-resolved microwave cond. expts.

L17 ANSWER 58 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1990:35401 Document No. 112:35401 2-Substituted-1-naphthols as potent 5-lipoxygenase inhibitors with topical antiinflammatory activity. Batt, Douglas G.; Maynard, George D.; Petraitis, Joseph J.; Shaw, Joan E.; Galbraith, William; Harris, Richard R. (Med. Prod. Dep., E. I. Du Pont de Nemours and Co. Inc., Wilmington, DE, 19880-0353, USA). J. Med. Chem., 33(1), 360-70 (English) 1990. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 112:35401; CJACS.

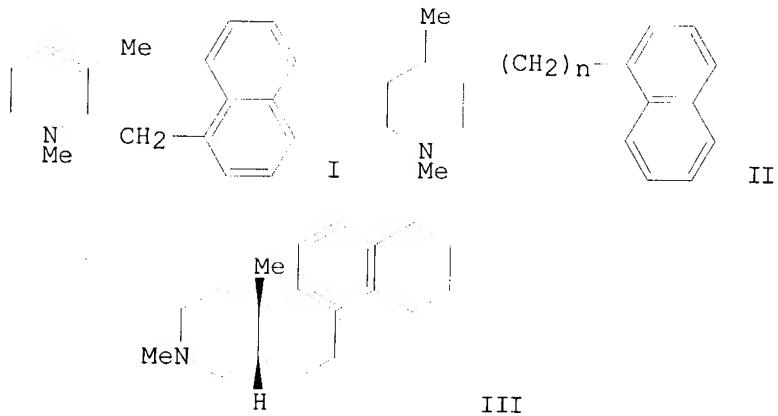
AB The synthesis, biol. evaluation, and structure-activity relationships of a series of 1-naphthols bearing carbon substituents at the 2-position are described. These compds. are potent inhibitors of the 5-lipoxygenase from

RBL-1 cells and also inhibit bovine seminal vesicle cyclooxygenase. Structure-activity relationships for these two enzymes are different, implying specific enzyme inhibition rather than a nonspecific antioxidant effect. 2-(Arylmethyl)-1-naphthols are among the most potent 5-lipoxygenase inhibitors reported (IC<sub>50</sub> values generally 0.1-0.2 .mu.M) and show excellent antiinflammatory potency in the mouse arachidonic acid ear edema model. To study the effects of structure on in vitro and in vivo activity, four general features of the mols. were varied: the 2-substituent, the 1-hydroxyl group, substitution on the naphthalene rings, and the 1,2-disubstituted naphthalene unit itself. 2-Benzyl-1-naphthol (DuP 654) shows a very attractive profile of topical antiinflammatory activity and is currently in clin. trials as a topically

applied antipsoriatic agent.

L17 ANSWER 59 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1989:533968 Document No. 111:133968 Intramolecular alkylations of aromatic compounds. XXV. The synthesis of hexahydro-7H-naphtho[1,8-fg]quinolines and -isoquinolines. Reimann, Eberhard; Hargasser, Eugen (Inst. Pharm. Lebensmittelchem., Univ. Muenchen, Munich, D-8000/2, Fed. Rep. Ger.). Arch. Pharm. (Weinheim, Ger.), 322(6), 363-7 (German) 1989. CODEN: ARPMA. ISSN: 0365-6233. OTHER SOURCES: CASREACT 111:133968.

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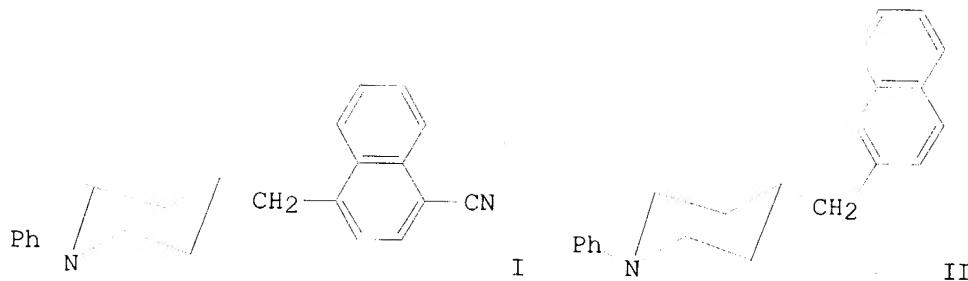
AB The carbinol prep. from 2-bromo-3-methylpyridine and 1-naphthaldehyde was oxidized to the ketone and reduced, quaternized, and reduced to give the tetrahydropyridine I which failed to cyclize. The isomer II ( $n = 1$ ) was prep. similarly and also failed to cyclize. Cyclization of II ( $n = 2$ ) gave the naphthoisooquinoline III.

L17 ANSWER 60 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1989:95011 Document No. 110:95011 Preparation and formulation of 2-(3-pyridylmethyl)naphthalene-6-carboxylic acid as a thromboxane synthetase inhibitor. Martinez, Gregory R.; Bruno, John J. (Syntex (U.S.A.), Inc., USA). U.S. US 4766127 A 19880823, 8 pp. (English). CODEN: USXXAM. APPLICATION: US 87-12979 19870210.

AB The title compd. (I), useful as thromboxane synthetase inhibitor in a mammal having a disease characterized by elevated thromboxane levels, was prep. 2-(3-Pyridylmethyl)-6-acetylnaphthalene, prep. in 6 steps from 2-bromonaphthalene, was converted via the haloform reaction to give I which gave 97.4% inhibition of human platelet aggregation at 2.0 times  $10^{-5}$  M. Tablets were prep. each contg. I 25, cornstarch 20, lactose 153, and Mg stearate 2 mg.

L17 ANSWER 61 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1989:23170 Document No. 110:23170 Intramolecular exciplex formation in jet-cooled, bichromophoric molecules. II. Dramatic effect of the acceptor electron affinity. Hermant, R. M.; Wegewijs, B.; Verhoeven, J. W.; Kunst, A. G. M.; Rettschnick, R. P. H. (Lab. Org. Chem., Univ. Amsterdam, Amsterdam, 1018 WS, Neth.). Recl. Trav. Chim. Pays-Bas, 107(4), 349-50 (English) 1988. CODEN: RTCPA3. ISSN: 0165-0513.

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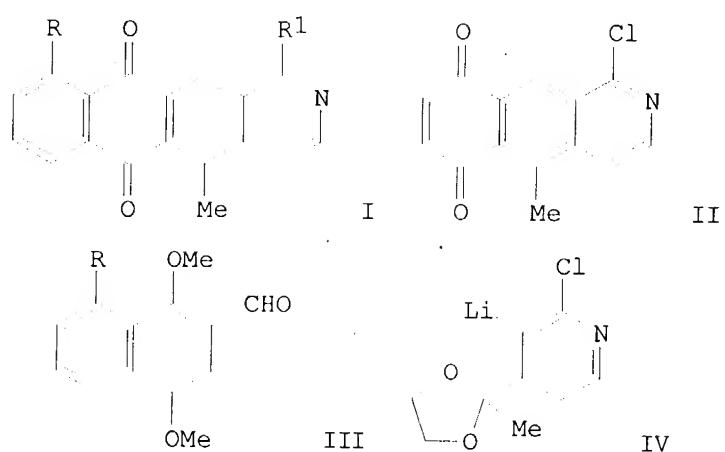
AB The jet-cooled fluorescence properties of two bichromophoric mols. (I and II), differing only in the acceptor chromophore, are compared. The barrier to exciplex formation in I, contg. a powerful cyanonaphthalene acceptor chromophore, is much lower than that in II which contains a less powerful naphthalene acceptor chromophore. It is thus proposed that the barrier is not only of a conformational nature, but also related to the energy required for intramol. charge sepn. in the Franck-Condon excited conformation which may then be followed by a fast, electrostatically-driven conformational change.

L17 ANSWER 62 OF 94 CAPLUS COPYRIGHT 1999 ACS

1988:590216 Document No. 109:190216 Synthesis of 1-functionalized 5-methylnaphtho[2,3-g]isoquinoline-6,11-quinones. Croisy-Delcey, Martine;

Rautureau, Marilyse; Huel, Christiane; Bisagni, Emile (Lab. Synth. Org., Inst. Curie, Orsay, 91405, Fr.). J. Org. Chem., 53(22), 5301-4 (English) 1988. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 109:190216; CJACS.

GI



AB 1-Chloro-5-methylnaphthoisoquinolinequinones I ( $R = H, OMe, OH; R1 = Cl$ ) were prep'd. by 2 independent pathways. Diels-Alder reaction of chloromethylbenzoisoquinolinequinone II with  $(E,E)-AcO(CH:CH)2OAc$  followed by aromatization gave I ( $R = H, R1 = Cl$ ). Addn. reaction of

IV 2-formyl-1,4-dimethoxynaphthalenes III (R = H, OMe) with lithiopyridine followed by a 1-pot redn.-hydrolysis-cyclization-dehydration-demethylation-oxidn. sequence (Et<sub>3</sub>SiH-CF<sub>3</sub>CO<sub>2</sub>H followed by aq. H<sub>2</sub>SO<sub>4</sub>) gave I (R = H, OMe, OH; R<sub>1</sub> = Cl). I (R = H, R<sub>1</sub> = Cl) reacted with amines to give I [R = H, R<sub>1</sub> = NHCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, NH(CH<sub>2</sub>)<sub>3</sub>NEt<sub>2</sub>, NH(CH<sub>2</sub>)<sub>3</sub>NMe<sub>2</sub>]; however, I (R = OH, OMe) gave only complex mixts. under similar conditions. I (R<sub>1</sub> = amino) were tested for cytotoxic and antileukemia activity (no data) but showed none.

L17 ANSWER 63 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1988:492810 Document No. 109:92810 Substituted pyridine derivatives, pharmaceutical preparations containing them, and their use in treating ulcers. Hosoi, Masaaki; Nishioka, Ryo; Hioki, Yoshio; Iida, Yoshiaki; Takeshita, Hiroshi; Niiyama, Kenji; Hidaka, Yusuke (Banyu Pharmaceutical Co., Ltd., Japan). Eur. Pat. Appl. EP 264883 A2 19880427, 47 pp.

DESIGNATED STATES: R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE.

(English). CODEN: EPXXDW. APPLICATION: EP 87-115275 19871019.

PRIORITY:

JP 86-248363 19861021; JP 87-199597 19870810.

GI For diagram(s), see printed CA Issue.

AB Pyridine derivs. I [R<sub>1</sub> = (un)substituted Ph or naphthyl; X = O, S, CO, CH(OH), NR<sub>a</sub> (Ra = H, alkyl); Y = alkylene, alkyl (un)substituted vinylene;

R<sub>2</sub>, R<sub>3</sub> = H, alkyl; R<sub>4</sub> = H, alkoxy, cycloalkyloxy, alkylthio, aryloxy, cycloalkylthio, aralkyloxy, NR<sub>b</sub>R<sub>c</sub> (R<sub>b</sub>, R<sub>c</sub> = H, alkyl; NR<sub>b</sub>R<sub>c</sub> = satd. heterocyclyl optionally with an addnl. hetero atom (O, S, N) and (un)substituted with alkyl); m, n = 0, 1, m and n .noteq. 0 simultaneously] or their acid addn. salts, useful in treating ulcers,

were

prepd. Wittig reaction of (1-naphthylmethyl)triphenylphosphonium chloride

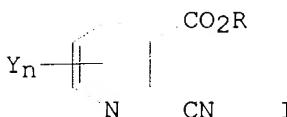
with 5-methyl-4-piperidino-2-pyridinecarboxaldehyde gave a mixt. of (E)- and (Z)-5-methyl-2-[2-(1-naphthyl)vinyl]-4-piperidinopyridines [(Z)-II], which was converted into 41% (E)- and 37% (Z)-II hydrochlorides (III). The ED<sub>50</sub> of III for gastric acid antisecretory activity was 1.16 mg/kg in rats. A formulation comprised III 200, lactose 70.3, potato starch 67.9, colloidal silica 12.8 g, and 10% aq. gelatin; after grinding and drying, potato starch 64, talc 20, and Mg stearate 2 g were added to give 4000 tablets each contg. 50 mg active compd.

L17 ANSWER 64 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1988:204503 Document No. 108:204503 Preparation of 2-cyanonicotinates as agrochemical fungicides. Lambert, Claude; Pepin, Regis (Rhone-Poulenc Agrochimie, Fr.). Eur. Pat. Appl. EP 246171 A2 19871119, 20 pp.

DESIGNATED STATES: R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE.

(French). CODEN: EPXXDW. APPLICATION: EP 87-420126 19870514. PRIORITY: FR 86-7260 19860516.

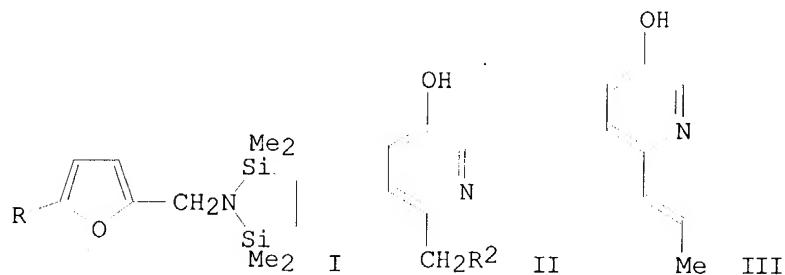
GI



AB The title compds. I [R = H, metal ion, (un)substituted ammonium, (un)substituted alkyl, alkenyl, alkynyl, Ph, pyridinylalkyl, etc.; Y = H, halo, alkyl, alkoxy; n = 1-3] were prep'd. 2-Cyanonicotinic acid was stirred with (Me<sub>2</sub>CH)<sub>2</sub>NH in Me<sub>2</sub>CO to give 99% I [R = (Me<sub>2</sub>CH)<sub>2</sub>NH<sub>2</sub>, Y = H] which, at .apprx.60 kg/ha applied to soil, gave at least 80% inhibition of *Piricularia oryzae* on rice.

L17 ANSWER 65 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1988:150268 Document No. 108:150268 Convenient syntheses of 6-arylmethyl- and 6-(1-E-propenyl)-3-pyridinols. Barrett, Anthony G. M.; Lebold, Suzanne A. (Dep. Chem., Northwestern Univ., Evanston, IL, 60208, USA). *Tetrahedron Lett.*, 28(47), 5791-2 (English) 1987. CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT 108:150268.

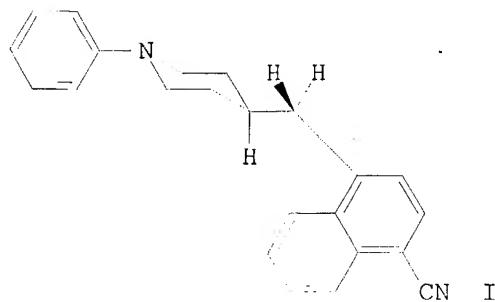
GI



AB Condensation reaction of (furylmethyl)azadisilacyclopentane I (R = Li), which was prep'd. by lithiation of I (R = H), with R<sub>1</sub>C<sub>6</sub>H<sub>4</sub>CHO (R<sub>1</sub> = H, 4-Me, 3-Me) or 2-naphthylaldehyde, followed by acid treatment gave phenylmethylpyridinols II (R<sub>2</sub> = Ph, C<sub>6</sub>H<sub>4</sub>Me-3, C<sub>6</sub>H<sub>4</sub>Me-4, 2-naphthyl) in 36-57% yields. The similar reaction of I (R = Li) with PhCHMeC(S)H gave II (R<sub>2</sub> = CHMeSPh) and pyridinol (E)-III.

L17 ANSWER 66 OF 94 CAPLUS COPYRIGHT 1999 ACS  
 1988:44260 Document No. 108:44260 Determination of the barrier to intramolecular exciplex formation in a jet-cooled, bichromophoric molecule. Wegewijs, B.; Hermant, R. M.; Verhoeven, J. W.; Kunst, A. G. M.; Rettschnick, R. P. H. (Lab. Org. Chem., Univ. Amsterdam, Amsterdam, 1018 WS, Neth.). *Chem. Phys. Lett.*, 140(6), 587-90 (English) 1987. CODEN: CHPLBC. ISSN: 0009-2614.

GI



AB The emissive properties of a bichromophoric mol. are reported. The mol. contains an anilino group as an electron donor (D) and a 1-cyanonaphthalene group as an electron acceptor (A) interconnected by a satd. hydrocarbon bridge of limited flexibility, which holds D and A far apart in the electronic ground state. The emission spectrum both in soln.

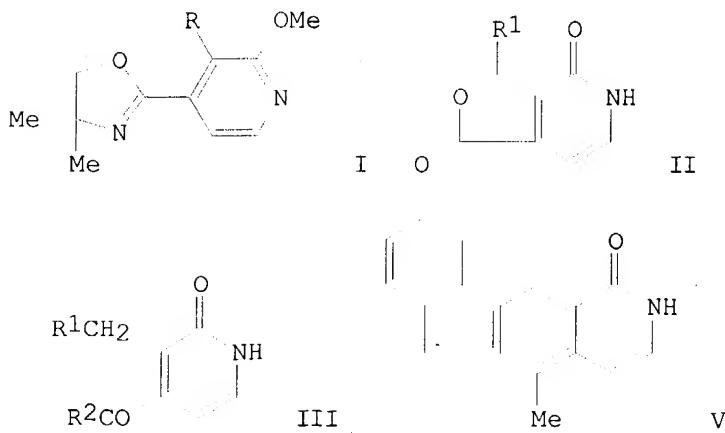
and in the gas phase, indicates that quant. formation of an intramol. exciplex between D and A occurs. This exciplex formation was studied as

function of excitation energy in a supersonic free jet. A barrier of  $1700.+-200$   $\text{cm}^{-1}$  was found between the Franck-Condon excited conformation and the conformation of the exciplex. Although this value is significantly higher than that reported earlier for exciplex formation between chromophores connected by a simple polymethylene chain ( $\text{apprxeq.} 900$   $\text{cm}^{-1}$ ) it is much lower than the barrier predicted for folding the bridge is sufficient to bring D and A in close contact. A tentative explanation of this discrepancy is given.

L17 ANSWER 67 OF 94 CAPLUS COPYRIGHT 1999 ACS

1988:21689 Document No. 108:21689 A new route to [g]-fused 5-methyl-1-functionalized isoquinolines. Bisagni, Emile; Rautureau, Marilys (Lab. Synth. Org., Inst. Curie, Orsay, F-91405, Fr.). Synthesis (2), 142-6 (English) 1987. CODEN: SYNTBF. ISSN: 0039-7881. OTHER SOURCES: CASREACT 108:21689.

GI



AB      Lithiated pyridyloxazoline I ( $R = Li$ ) condensed with  $R_1 CHO$  ( $R_1 = 1-, 2-, 3-$ substituted phenyl,  $n = 1, 2$ )

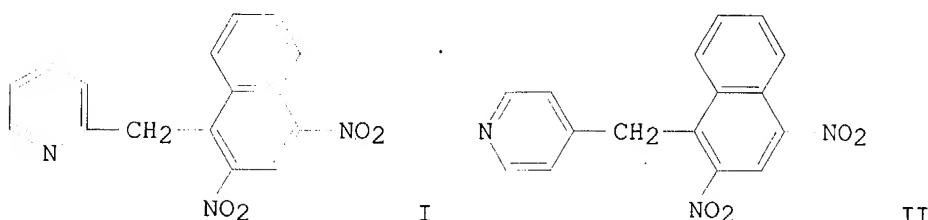
2-naphthyl, m-MeOC<sub>6</sub>H<sub>4</sub>, 3-thienyl) to give 62-75% I [R = R<sub>1</sub>CH(OH)], hydrolysis of which with 4N HCl gave 68-91% lactones II. Redn. of II with

Zn(NH<sub>3</sub>) or catalytic hydrogenation over Pd gave 61-78% carboxylic acids III (R<sub>2</sub> = OH), which, with MeLi, gave 19-69% III (R<sub>2</sub> = Me) (IV). Acidic ring closure of IV easily gave 43-71% title compds. such as V.

L17 ANSWER 68 OF 94 CAPLUS COPYRIGHT 1999 ACS

1987:597398 Document No. 107:197398 Photochromism of (nitronaphthyl)methyl derivatives of pyridine. Ponyaev, A. I.; Ol'khovskii, V. V.; Zakhs, E. R.; El'tsov, A. V. (Leningr. Tekhnol. Inst., Leningrad, USSR). Zh. Org. Khim., 22(10), 2217-22 (Russian) 1986. CODEN: ZORKAE. ISSN: 0514-7492.

GI

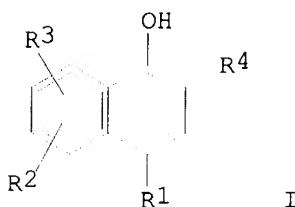


AB Photolysis of title compds. I and II in aq. EtOH produced colored azamerocyanine or azamerocyanine anion forms, depending on the pH. For II, the equil. const. pKa = 6.4 between the colored forms was detd. Decoloration of the colored forms of I and II was a pseudo first-order process, and the rate consts. were almost 2 orders of magnitude smaller than those of the corresponding (dinitrobenzyl)pyridines.

L17 ANSWER 69 OF 94 CAPLUS COPYRIGHT 1999 ACS

1987:452007 Document No. 107:52007 2-Substituted-1-naphthols as 5-lipoxygenase inhibitors. Batt, Douglas Guy (du Pont de Nemours, E. I., and Co., USA). Eur. Pat. Appl. EP 201071 A2 19861112, 87 pp. DESIGNATED STATES: R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 86-106122 19860505. PRIORITY: US 85-731791 19850508; US 86-839912 19860319.

GI



AB Naphthol derivs. I [R<sub>1</sub> = H, Me, Br, Cl, OH, OMe, OEt, Ph, S, SO, SO<sub>2</sub>, (un)substituted NH<sub>2</sub>, etc.; R<sub>2</sub>, R<sub>3</sub> = H, Me, Et, OMe, OEt; R<sub>4</sub> = alkyl, alkenyl, alkynyl, etc.] are prep'd. as 5-lipoxygenase inhibitors. Thus, 1,1,1-trimethoxy-5-hexyne in dry THF was treated at -78.degree. with BuLi in hexane, followed by the addn. of 1-benzyloxy-2-naphthaldehyde in THF, to give Me 7-(1-benzyloxy-2-naphthyl)-7-hydroxy-5-heptynoate. This was treated with a mixt. of BF<sub>3</sub>.Et<sub>2</sub>O, Et<sub>3</sub>SiH, and CH<sub>2</sub>C<sub>12</sub> to give Me 7-(1-benzyloxy-2-naphthyl)-5-heptynoate, which, upon treatment with EtSH

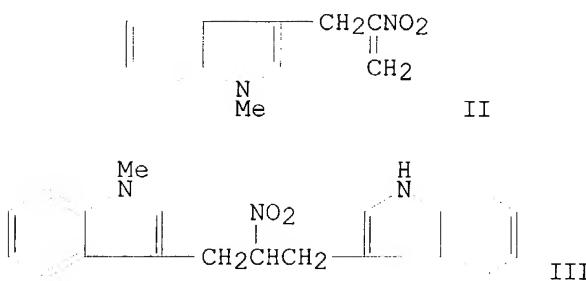
and  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  gave I ( $\text{R}_1 = \text{R}_2 = \text{R}_3 = \text{H}$ ,  $\text{R}_4 = \text{CH}_2\text{C}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}_2\text{Me})$ ).

L17 ANSWER 70 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1984:406584 Document No. 101:6584 2-Nitro-2-propen-1-yl 2,2-dimethylpropanoate (NPP), a multiple coupling reagent. Seebach, Dieter; Knochel, Paul (Lab. Org. Chem., Edig. Tech. Hochsch. Zurich, Zurich, CH-8092, Switz.). *Helv. Chim. Acta*, 67(1), 261-83 (English) 1984.

CODEN:

HCACAV. ISSN: 0018-019X.

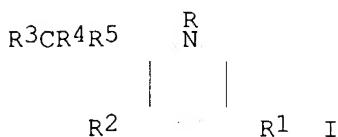
GI



AB The title compd.,  $\text{H}_2\text{C}(\text{NO}_2)\text{CH}_2\text{O}_2\text{CCMe}_3$  (I), prep'd. from  $\text{HCHO}$ ,  $\text{MeNO}_2$ , and  $\text{Me}_3\text{CCOCl}$ , is a versatile nitroallylating reagent which combines with nucleophiles as different as anilines, indoles, enolates, and organolithium compds. Some 40 examples were given. Thus, adding I to  $\text{PhNHMe}$  at -78. $^\circ$  and stirring 2 h gave 86%  $\text{PhNMeCH}_2\text{C}(\text{NO}_2):\text{CH}_2$ . Thirteen examples of the addn. of 2 different nucleophiles to the C3 moiety of I were described. I is useful as a multiple coupling reagent for convergent syntheses, even of products not contg.  $\text{NO}_2$  groups. Thus, propenylindole II, prep'd. from I and N-methylindole, reacted with indole to give diindole III.

L17 ANSWER 71 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1984:174627 Document No. 100:174627 Piperidine derivatives. Dixon, J.; Robinson, D. H. (USA). *Res. Discl.*, 238, 49-50 (English) 1984. CODEN: RSDSBB. ISSN: 0374-4353.

GI



AB Piperidines I [ $\text{R} = \text{H}$ , alkyl, alkenyl, cycloalkylalkenyl, aralkyl, pyridylalkyl;  $\text{R}_1, \text{R}_3, \text{R}_4 = \text{H}$ , alkyl;  $\text{R}_2 = \text{H}, \text{OH}$ ;  $\text{R}_5 = (\text{un})\text{substituted Ph}$ , naphthyl, fluorenyl] were prep'd. I affect heart rate (no data).

L17 ANSWER 72 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1984:6025 Document No. 100:6025 Thermolyses and reactions of 4,5-benzotricyclo[4.1.0.01,3]-hept-4-ene and o-(propadienyl)styrene. Brinker, Udo H.; Wilk, Gabriele; Gomann, Klaus (Abt. Chem., Ruhr-Univ., Bochum, 4630/1, Fed. Rep. Ger.). *Angew. Chem.*, 95(11), 892-3 (German)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The benzotricycloheptene I and propadienylstyrene II underwent thermolysis

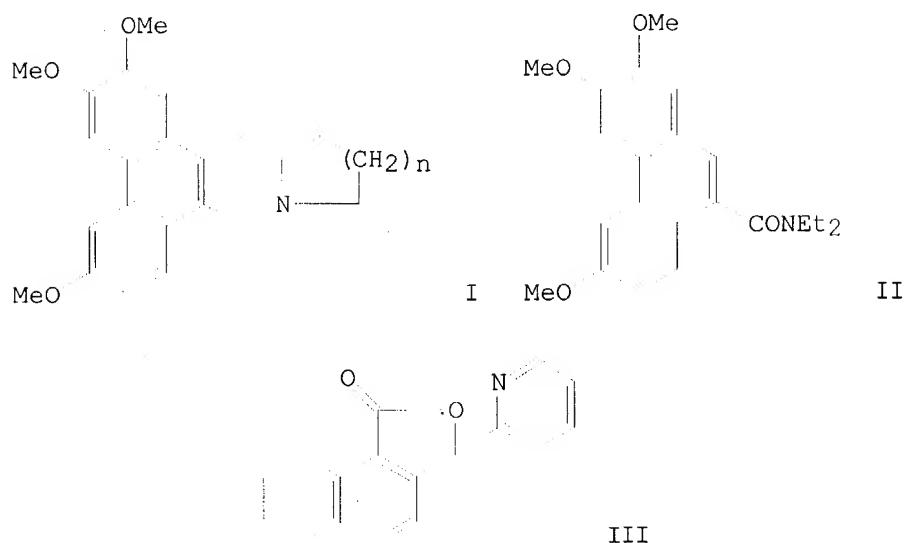
at 30.degree. to give adducts III and IV and 2-methylnaphthalene via cycloaddn. of intermediate V. The thermolysis kinetics was detd. and the mechanism discussed. I and II reacted with N-phenylmaleimide at 52.2.degree. to give the adducts VI and VII. I and II also gave adducts with (CN)2C:C(CN)2 at 60.degree..

L17 ANSWER 73 OF 94 CAPLUS COPYRIGHT 1999 ACS

1983:540204 Document No. 99:140204 Directed ortho metalation of tertiary aromatic amides. A new N-hetero ring annelation method and synthesis of phenanthroquinolizidine and -indolizidine alkaloids. Iwao, M.; Mahalanabis, K. K.; Watanabe, M.; De Silva, S. O.; Snieckus, V. (Guelph-Waterloo Cent. Grad. Work Chem., Univ. Waterloo, Waterloo, ON,

N2L 3G1, Can.). Tetrahedron, 39(12), 1955-62 (English) 1983. CODEN: TETRAB. ISSN: 0040-4020.

GI

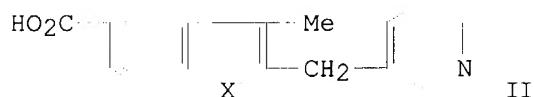


AB The synthesis of the phenanthro-quinolizidine and -indolizidine alkaloids cryptopleurine (I, n = 2) and antofine (I, n = 1) via directed ortho metalation of the common phenanthrene II are described. The utility of this strategy as a new N-hetero ring annelation method is illustrated by the prepn. of other arom. ring-fused quinolizidine and indolizidine systems. A Mg for Li transmetalation, crucial for the synthesis of III and of potential broader significance in directed metalation chem., is reported.

L17 ANSWER 74 OF 94 CAPLUS COPYRIGHT 1999 ACS

1983:505247 Document No. 99:105247 Thromboxane synthetase inhibitors, and pharmaceutical compositions comprising them. Cross, Peter Edward; Dickinson, Roger Peter (Pfizer Ltd., UK; Pfizer Corp.). Eur. Pat. Appl. EP 73663 A2 19830309, 121 pp. DESIGNATED STATES: R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 82-304528 19820826. PRIORITY: GB 81-25976 19810826.

GI

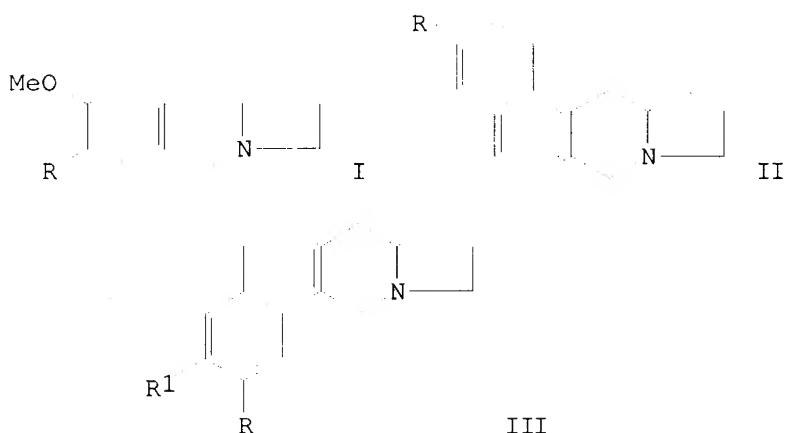


AB Imidazoles I (R = Me, Cl, SMe, H; X = O, S, NMe), the pyridines II (X = X, CH:CH), and related compds. (29 compds.) were prep'd. Thus Et 3-methyl-5-benzothiophenecarboxylate was chloromethylated, treated with imidazole, and hydrolyzed to give I (R = Me, X = S) which at 0.1 mg/kg i.v. in rabbits gave 100% inhibition of thromboxane B<sub>2</sub> prodn.

L17 ANSWER 75 OF 94 CAPLUS COPYRIGHT 1999 ACS

1982:492106 Document No. 97:92106 Synthesis of hexahydropyrrolo[1,2-b]isoquinolines - analogs of phenanthroindolizidine anticancer alkaloids. Gaur, S. P.; Jain, Padam C.; Anand, Nitya (Med. Chem. Div., Cent. Drug Res. Inst., Lucknow, 226 001, India). Indian J. Chem., Sect. B, 21B(1), 46-51 (English) 1982. CODEN: IJSBDB. ISSN: 0376-4699.

GI

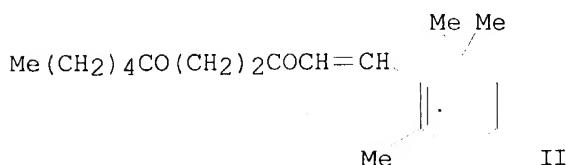


AB A convenient preparative route was developed for the synthesis of hexahydropyrrolo[1,2-b]isoquinolines involving condensation of an aryl aldehyde with Et 4-nitrobutanoate followed by LiAlH<sub>4</sub> redn. and subsequent cyclization with H<sub>2</sub>SO<sub>4</sub> to 2-arylmethylpyrrolidines. The latter on formylation and Bischler-Napieralski cyclization followed by NaBH<sub>4</sub> redn.

gave the required pyrroloisoquinolines. Using this method, pyrroloisoquinolines I ( $R = H, MeO$ ), benzopyrroloisoquinolines II ( $R = H, MeO$ ), and III ( $R = H, R1 = H, MeO; R = R1 = MeO$ ) were synthesized. None of the compds. showed any noteworthy anticancer activity, while only few exhibited antihistaminic,  $\beta$ -blocking, hypertensive, antiinflammatory, and antireserpine activities.

L17 ANSWER 76 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1982:19258 Document No. 96:19258 Nitroallylation of highly reactive  
organolithium compounds by 2-nitro-3-pivaloyloxy-1-propene (NPP).  
Knochel, Paul; Seebach, Dieter (Lab. Org. Chem., Eidg. Tech. Hochsch.,  
Zurich, CH-8092, Switz.). *Tetrahedron Lett.*, 22(34), 3223-6 (English)  
1981. CODEN: TELEAY. ISSN: 0040-4039.

GI

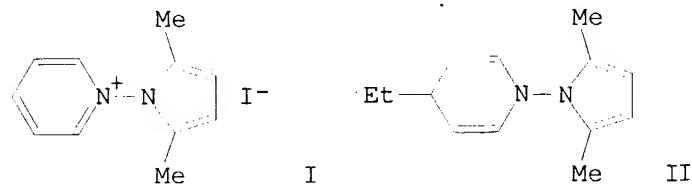


AB CH<sub>2</sub>:C(NO<sub>2</sub>)CH<sub>2</sub>O<sub>2</sub>CCMe<sub>3</sub> (NPP) efficiently transfers a CH<sub>2</sub>:C(NO<sub>2</sub>)CH<sub>2</sub> group to even the most reactive nucleophilic centers of organolithium reagents (RLi) to give high yields of products RCH<sub>2</sub>C(:CH<sub>2</sub>)NO<sub>2</sub>. E.g., NPP reacted with BuLi or Ph(CH<sub>2</sub>)<sub>2</sub>Cl (THF, -70 to -110.<sup>o</sup>.) to give 77% Me(CH<sub>2</sub>)<sub>4</sub>C(:CH<sub>2</sub>)NO<sub>2</sub> (I) and 68% Ph(CH<sub>2</sub>)<sub>3</sub>C(:CH<sub>2</sub>)NO<sub>2</sub>, resp. Reaction of I with  $\beta$ -ionone, followed by Nef-reaction gave the 1,4-diketone II in high yield.

L17 ANSWER 77 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1981:515216 Document No. 95:115216 Synthetic applications of  
nitrogen-nitrogen linked heterocycles. Part 13.

N-(2,5-dimethylpyrrol-1-yl)pyridinium salts in the synthesis of 4-alkyl- and 4-arylpyridines via regiospecific attack of Grignard reagents and organolithium compounds. Katritzky, Alan R.; Beltrami, Hector; Sammes, Michael P. (Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA). J. Chem. Res., Synop. (5), 133 (English) 1981. CODEN: JRPSDC. ISSN: 0308-2342.

GI



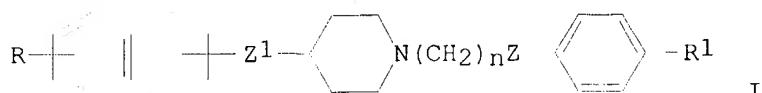
AB Reaction of N-(2,5-dimethylpyrrol-1-yl)pyridinium iodides and Grignard reagents or diorganolithium compds. gave 1,4-dihydrointermediates regiospecifically. Decomprn. of these under free radical conditions gave moderate to good yields of 4-substituted pyridines. E.g., I was treated with  $\text{Et}_2\text{MgBr}$  ( $\text{P} = \text{halide}$ ) ( $\text{THF}, 25^\circ\text{C}$ ) to give 77% II

## WITH ELMGR 4-Ethylpyridine

72 was obtained from II (39%) on decompr. [Me2C(CN)N:NCMe2CN, THF, reflux,  
h].

L17 ANSWER 78 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1981:30578 Document No. 94:30578 4-(Naphthylmethyl)-piperidine derivatives.  
Carr, Albert A. (Richardson-Merrell Inc., USA). Ger. Offen. DE 3002292  
19800821, 57 pp. (German). CODEN: GWXXBX. PRIORITY: US 79-10555  
19790209.

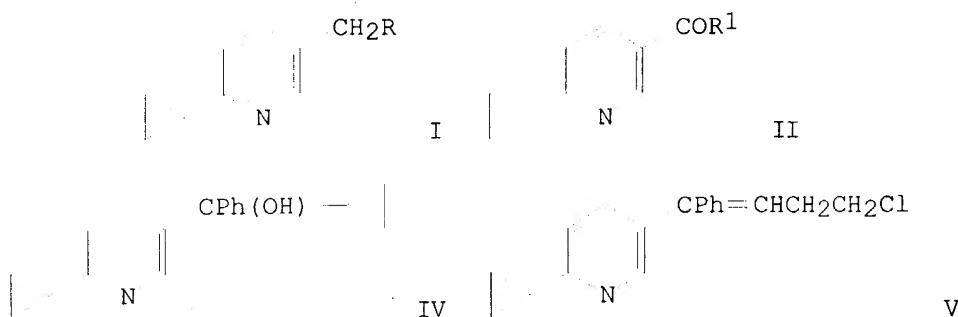
GI



AB The title compds. I ( $n = 2-5$ ; R = H, halo, C1-4 alkyl or alkoxy, CF<sub>3</sub>; R<sub>1</sub> = H, halo, C1-4 alkyl or alkoxy; Z = CO, CHO<sub>H</sub>; Z<sub>1</sub> = CO, CHO<sub>H</sub>, CH<sub>2</sub>) were prep'd. for use as neuroleptic tranquilizers. Thus, Friedel-Crafts acylation of C10H<sub>8</sub> with 4-piperidinecarbonyl chloride gave 2-naphthyl 4-piperidyl ketone-HCl, which reacted with Cl(CH<sub>2</sub>)<sub>3</sub>COPh in the presence of KHCO<sub>3</sub> to give I (R = R<sub>1</sub> = H, Z = Z<sub>1</sub> = CO, n = 3, 2-naphthyl).

L17 ANSWER 79 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1980:446428 Document No. 93:46428 2-Cyclopropyl-5-substituted pyridines.  
Miyano, Koichi; Sakai, Taketsugu; Hamano, Hiroaki (Nippon Kayaku Co.,  
Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 54157568 19791212 Showa, 9 pp.  
(Japanese). CODEN: JKXXXAF. APPLICATION: JP 78-63322 19780529.

GI



AB      Seventeen title compds. I (R = alkyl, cyclohexyl, haloalkyl, Ph, substituted Ph, naphthyl) were prep'd. starting with II (R<sub>1</sub> = cyclopropyl) (III). Thus, 19.7 g III in THF was added to PhMgBr in THF at 5-30.degree.

and the mixt. stirred 3 h at room temp. to give 29.9 g IV, which (29 g) was dissolved in C6H6, 100 mL concd. HCl added at <30.degree., and the mixt. stirred 15 h at room temp. to give 29.5 g V, which (27.5 g) was oxidized with KMnO4 in Me2CO at 40-50.degree. to give 95% II (R1 = Ph), which (12.2 g) was reduced to give 88% I (R = Ph), converted to the

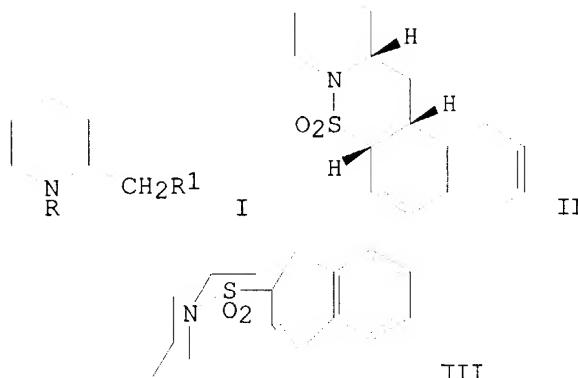
picrate.

L17 ANSWER 80 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1977:584378 Document No. 87:184378 3-Substituted 3-ethoxycarbonyl-2-piperidones. Kikumoto, Ryoji; Okubo, Kazuo (Mitsubishi Chemical Industries Co., Ltd., Japan). Japan. Kokai JP 52083671 19770712 Showa, 3 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 76-223 19760101.  
GI For diagram(s), see printed CA Issue.  
AB Title compds. I [R = Ph, 1-naphthylmethyl, PhCH<sub>2</sub>, 2-(1-naphthyl)ethyl] were prep'd. by catalytic redn. of NCCH<sub>2</sub>CH<sub>2</sub>CR(CO<sub>2</sub>Et)<sub>2</sub>. Thus, a mixt. of 8.67 g NCCH<sub>2</sub>CH<sub>2</sub>CPh(CO<sub>2</sub>Et)<sub>2</sub>, 0.4 g Ni-SiO<sub>2</sub>, and 80 kg/cm<sup>2</sup> H in EtOH was shaken 5 h at 100.degree. to give 69% I (R = Ph).

L17 ANSWER 81 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1977:584018 Document No. 87:184018 2-Substituted-5-aminovaleric acids. Kikumoto, Ryoji; Okubo, Kazuo (Mitsubishi Chemical Industries Co., Ltd., Japan). Japan. Kokai JP 52083602 19770712 Showa, 3 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 76-221 19760101.  
GI For diagram(s), see printed CA Issue.  
AB Four title acids H<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>CHRCO<sub>2</sub>H I [R = Ph, 1-naphthylmethyl, 2-(1-naphthyl)ethyl, PhCH<sub>2</sub>] were prep'd. by hydrolysis of piperidones II. Thus, stirring II (R = Ph) with 40% aq. H<sub>2</sub>SO<sub>4</sub> 4 h at 110.degree. gave 89.1% I (R = Ph).

L17 ANSWER 82 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1977:535160 Document No. 87:135160 Formation of a 1,2-dihydronaphthalene via methylene radical attack on a naphthalene nucleus. Koehler, J. J.; Speckamp, W. N. (Lab. Org. Chem., Univ. Amsterdam, Amsterdam, Neth.). Tetrahedron Lett. (7), 635-8 (English) 1977. CODEN: TELEAY.

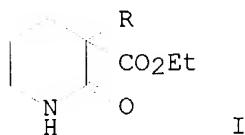
GI



AB Iodide I (R = O<sub>2</sub>SC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-4, R<sup>1</sup> = I) with Bu<sub>3</sub>SnH gave 56% rearranged product I (R = H, R<sup>1</sup> = 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>). I [R = O<sub>2</sub>SR<sup>2</sup> (R<sup>2</sup> = 3-pyridyl), R<sup>1</sup> = I] underwent redn. and rearrangement to give I (R = O<sub>2</sub>SR<sup>2</sup>, R<sup>1</sup> = H; R = H, R<sup>1</sup> = 3-pyridyl). Naphthyl sulfonamide I (R = O<sub>2</sub>SC<sub>10</sub>H<sub>7</sub>-2, R<sup>1</sup> = I) with Bu<sub>3</sub>SnH gave 13% rearranged product I (R = H, R<sup>1</sup> = 2-C<sub>10</sub>H<sub>7</sub>) and 81% 1,6-addn. product II. II is formed by H transfer via radical intermediate III.

L17 ANSWER 83 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1977:517782 Document No. 87:117782 3-Substituted-3-ethoxycarbonyl-2-piperidinones. Kikumoto, Ryoji; Okubo, Kazuo (Mitsubishi Chemical Industries Co., Ltd., Japan). Japan. Kokai JP 52010277 19770126 Showa, 3 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 75-86086 19750714.

GI



AB Four 3-substituted-3-ethoxycarbonyl-2-piperidones I (R = Ph, .alpha.-naphthylmethyl, PhCH<sub>2</sub>, .alpha.-naphthylethyl) were prepd. by redn. of Et .alpha.-substituted-.alpha.- (2-cyanoethyl)malonates NCCH<sub>2</sub>CH<sub>2</sub>CR(CO<sub>2</sub>Et)<sub>2</sub> in the presence of H-activating catalysts. Thus, a mixt. of 8.67 g NCCH<sub>2</sub>CH<sub>2</sub>C<sub>6</sub>H<sub>5</sub>(CO<sub>2</sub>Et)<sub>2</sub>, 0.4 g Ni-SiO<sub>2</sub>, and 80 kg/cm<sup>2</sup> H in EtOH was autoclaved 5 h at 100.degree. to give 69% I (R = Et).

L17 ANSWER 84 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1975:514691 Document No. 83:114691 Synthesis of 2,5-dimethyl-6,7-naphthomorphan. Pandey, R. K.; Joshi, B. C. (Chem. Lab., Univ. Rajasthan, Jaipur, India). Bull. Acad. Pol. Sci., Ser. Sci. Chim., 23(5), 385-7 (English) 1975. CODEN: BAPCAQ.

GI For diagram(s), see printed CA Issue.

AB The title compd. I was prepd. from the dihydropyridine II by successive NaBH<sub>4</sub> redn. and cyclization in 48% HBr. II was prepd. by reaction of 4-picoline methiodide with (1-naphthylmethyl)magnesium chloride.

L17 ANSWER 85 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1973:452822 Document No. 79:52822 Glutaric acid imides. Kirchlechner, Richard; Seubert, Juergen; Rogalski, Werner (Merck Patent G.m.b.H.).  
Ger. Offen. DE 2141946 19730301, 44 pp. (German). CODEN: GWXXBX.  
APPLICATION: DE 71-2141946 19710821.  
GI For diagram(s), see printed CA Issue.  
AB About 31 glutarimides (I; R = H, Me, Pr; R<sub>1</sub> = H, Me; R<sub>2</sub> = H, MeO, Cl; R<sub>3</sub> = H, MeO; R<sub>3</sub>R<sub>4</sub> = benzo, etc.) were prepd. by various methods. E.g., C<sub>6</sub>H<sub>4</sub>(OMe)<sub>2</sub>-p with succinic anhydride in the presence of AlCl<sub>3</sub> gave 2,5-(MeO)C<sub>6</sub>H<sub>3</sub>COCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, which with HCOCO<sub>2</sub>H gave HO<sub>2</sub>CCH<sub>2</sub>C[COC<sub>6</sub>H<sub>3</sub>(MeO)<sub>2</sub>-2,5]CH<sub>2</sub>CO<sub>2</sub>H, redn. of this gave HO<sub>2</sub>CCH<sub>2</sub>CH[CH<sub>2</sub>C<sub>6</sub>H<sub>3</sub>(MeO)<sub>2</sub>-2,5]CH<sub>2</sub>CO<sub>2</sub>H, which was heated with NH<sub>3</sub> 1 hr at 160.degree. and 30 min at 160-70.degree. to give I (R, R<sub>1</sub>, R<sub>4</sub> = H; R<sub>2</sub>, R<sub>3</sub> = MeO).

L17 ANSWER 86 OF 94 CAPLUS COPYRIGHT 1999 ACS  
1973:147664 Document No. 78:147664 Oxocarboxylic acids and amides. Kirchlechner, Richard; Rogalskii, Werner; Seubert, Juergen (Merck Patent G.m.b.H.). Ger. Offen. DE 2141947 19730301, 39 pp. (German). CODEN: GWXXBX. APPLICATION: DE 71-2141947 19710821.  
AB (Tetrahydrooxonaphthyl)acetamides (I, R=H or 1 more halogen, MeO, OH, and/or Me groups; R<sub>1</sub>=H, Me, Pr; R<sub>2</sub>=H, Me) were prepd. by treating a 3-(substituted benzyl)glutarimide with a mineral acid and/or a

Friedel-Crafts catalyst. Thus, 3-(2-chloro-5-methoxybenzyl)-3-methylglutarimide with HF gave I (R=5-Cl, 8-MeO; R1=Me; R2=H), and 3-(3-methoxybenzyl)glutarimide with AlCl<sub>3</sub> gave I (R=6-MeO, R1, R2=H). Several I were hydrolyzed in the presence of base to give the corresponding naphthaleneacetic acids. 3-(1-Naphthylmethyl)glutarimide with HF gave 2-(1,2,3,4-tetrahydro-1-oxo-3-phenanthryl)acetamide.

L17 ANSWER 87 OF 94 CAPLUS COPYRIGHT 1999 ACS

1972:428268 Document No. 77:28268 Acidic zinc fluoborate electrolyte for a zinc electroplating process. Page, Walter; Schevey, William R.; Van der Mey, John E. (Allied Chemical Corp.). U.S. US 3655533 19720411, 7 pp. (English). CODEN: USXXAM. APPLICATION: US 70-89068 19701112.

AB Ferrous metal impurities which get into acidic fluoroborate plating baths through corrosive action of the bath on the base metal, etc., are prevented from reducing the quality of the Zn plating by codepositing with the Zn, by adding to the bath a mixt. of (1) a 4-hydroxy-, 4-alkyl- or aryl-, 5-acyl- or aroylpiperidine and (2) thiourea or N-substituted deriv.

thereof. Thus, to 1 set of a series of baths contg. Zn(BF<sub>4</sub>)<sub>2</sub> 300, NH<sub>4</sub>Cl 30, and NH<sub>4</sub>BF<sub>4</sub> 12 g/l., adjusted to pH 3-3.5 with NH<sub>4</sub>OH, there is added 0.25 g/l. of a com. mixt. contg. 70% of an inert inorg. salt filler and 30% of a mixt. of 66.7 % of a substituted piperidine compd. and 33.3% of (p-MeC<sub>6</sub>H<sub>4</sub>NH)<sub>2</sub>CS. The baths with the addnl. mixts. have .apprx.300% greater tolerance for Fe which is exptl. added to the baths as Fe(BF<sub>4</sub>)<sub>2</sub>.

L17 ANSWER 88 OF 94 CAPLUS COPYRIGHT 1999 ACS

1971:87902 Document No. 74:87902 Dianions derived from glutarimide, 3,5-morpholinedione, and 3,5-thiomorpholinedione as useful new synthetic intermediates. Wolfe, James F.; Rogers, Tommie Gene (Dep. Chem.,

Virginia Polytech. Inst., Blacksburg, Va., USA). J. Org. Chem., 35(11), 3600-7 (English) 1970. CODEN: JOCEAH.

AB Glutarimide (I), 3,5-mor-pholinedione (II), and 3,5-thiomorpholinedione (III) were con-verted to their resp. dianions by means of slightly more than 2 molar equiv. NaNH<sub>2</sub> in liq. NH<sub>3</sub>. Reactions of the dianions de-ived

from I and II with alkyl halides and carbonyl compds. afforded .alpha.-substituted derivs. of the parent heterocycles. The dianion of III gave a similar monosubstituted deriv. on treatment with MeOBz but underwent a dicondensation reaction with benzophenone and polyalkylation with BuBr. Satisfactory monoalkylation at the .alpha. carbon of III was accomplished when Li-NH<sub>2</sub> was used to generate the dianion. Synthetically useful yields were obtained in a majority of the reactions of these new dianions.

L17 ANSWER 89 OF 94 CAPLUS COPYRIGHT 1999 ACS

1970:445374 Document No. 73:45374 Anticonvulsant 1,2,5,6-tetrahydropyridine and 1,2-dihydropyridine derivatives. Albertson, Noel F. (Sterling Drug Inc.). U.S. US 3514461 19700526, 4 pp. Continuation-in-part of U.S. 3382249 (English). CODEN: USXXAM. APPLICATION: US 19670912.

AB The title compds. were prep'd. and used as intermediates for prepg. anticonvulsant, analgesic, and antagonist naphthazocines. N,3,4-Trimethyl-2-(1-naphthylmethyl)-1,2-dihydropyridine, prep'd. by treating 1-naphthylmethylmagnesium chloride with 3,4-dimethylpyridine methiodide, was reduced with NaBH<sub>4</sub> to give N,3,4-trimethyl-2-(1-naphthylmethyl)-1,2,5,6-tetrahydropyridine (I). A mixt. of I and HBr was refluxed, the product partitioned between H<sub>2</sub>O and EtOAc, the aq. layer made alk., and extd. to give racemic 1,2,3,4,5,6-hexahydro-3-methyl-6,13-dimethyl-2,6-methano-3-naphth[2,1-f]azocine, which was converted to racemic 1,2,3,4,5,6-hexahydro-cis-6,13-dimethyl-2,6-methano-3-naphth[2,1-

f]azocine by treating with CNBr and refluxing with concd. HCl.

L17 ANSWER 90 OF 94 CAPLUS COPYRIGHT 1999 ACS

1968:496509 Document No. 69:96509 Benzazocines and Naphthazocines.

Albertson, Noel F. (Sterling Drug Inc.). U.S. US 3382249 19680507, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 19641020.

GI For diagram(s), see printed CA Issue.

AB The title compounds, useful as anticonvulsants and analgesic antagonists, are prep'd. by multi-step syntheses. Thus, a soln. of 274 g.  $\alpha$ -C<sub>10</sub>H<sub>7</sub>CH<sub>2</sub>Cl in 1250 ml. Et<sub>2</sub>O is added slowly to a mixt. of 258 ml. Et<sub>2</sub>O and 37.2 g. Mg turnings, the liq. is siphoned into a soln. of 376 g. 3,4-dimethylpyridine-MeI in 1500 ml. Et<sub>2</sub>O, the mixt. stirred 10 min., poured into ice-NH<sub>4</sub>OH, treated with 500 ml. concd. NH<sub>4</sub>OH and the Et<sub>2</sub>O layer sepd. and evapd., giving 267 g. oily 2-(1-naphthylmethyl)-1,3,4-trimethyl-1,2-dihydropyridine, redn. of which in 1 l. EtOH with 28 g. NaBH<sub>4</sub> in 240 ml. H<sub>2</sub>O at 15-20.degree. 4 hrs. gives 148 g. of the tetrahydro deriv. (I), b0.2-0.6 148-56.degree.. Refluxing 147 g. I with 1500 ml. 48% HBr 24 hrs. gives 134 g. dark oil which crystallizes from

100

ml. chilled Me<sub>2</sub>CO as 89.9 g. II, (R = Me) (III), m. 55-73.degree., separable by chromatog. into cis (m. 81.degree.) and trans (m. 135.degree.) isomers. A soln. of 42 g. cis-III in 210 ml. CHCl<sub>3</sub> is added dropwise at room temp. to a soln. of 17 g. CNBr in 170 ml. CHCl<sub>3</sub>, the mixt. is refluxed 3 hrs., evapd., 105 ml. concd. HCl and 535 ml. H<sub>2</sub>O is added, the mixt. is refluxed 24 hrs. giving 28.1 g. cis-II (R = H) (IV), b0.4-0.6 151-4.degree.; hydrochloride m. 283-7.degree.. Similarly, 15 g. of trans-III gives 8.5 g. trans-IV, b0.5 153-6.degree.; hydrochloride m. 329-37.degree.. To 8.3 g. cis-IV and 5 ml. Et<sub>3</sub>N in 50 ml. CHCl<sub>3</sub> is added 3.6 g. cyclopropylcarbonyl (A) chloride in 25 ml. CHCl<sub>3</sub>, giving 10 g. cis-II (R = A) (V), an oil, which is reduced by 3 g. LiAlH<sub>4</sub> in 150 ml. tetrahydrofuran to 5 g. cis-II [R = cyclopropylmethyl-(B)] (VI), m. 78-81.degree.. Similarly, 7.4 g. trans-IV gives 4 g. trans-V, m. 134-6.degree., which is converted to trans-VI; hydrochloride m. 249-52.degree.; and 8.3 g. cis-IV is converted to 5.7 g. cis-II [R = cyclobutylmethyl(C)], m. 80-3.degree., via 11.2 g. cis-II (R = cyclobutylcarbonyl). Using the above methods, the following derivs. of cis-and trans-VII (R<sub>2</sub> = H) are prep'd. (given are geometrical isomer, R<sub>1</sub>, g. starting material, R<sub>2</sub>, g. product, salt m.p. or b.p./mm. of product): cis, Me, 8, B, 6.8, 119-22.degree./0.8 (HCl m. 249-51.degree.); trans,

Me,

6, B, 3.1, HBr 238-40.degree.; cis, Et, 9, B, 3.8, HCl 243-9.degree.;

cis,

Me, 5.8, C, 5.3, HCl 270-1.degree.; cis, Me, -, 3,3-dimethylcyclobutylmethyl, 9.3, HCl 240-1.degree.; cis, Me, 8, cyclopentylamethyl, 6.0, HCl 246-9.degree..

L17 ANSWER 91 OF 94 CAPLUS COPYRIGHT 1999 ACS

1968:467158 Document No. 69:67158 Stereochemistry of aziridine formation by reduction of oximes with lithium aluminum hydride on aralkyl alkyl ketoximes and their tosylates. Kotera, K.; Okada, T.; Miyazaki, S. (Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, Japan). Tetrahedron, 24(16), 5677-90 (English) 1968. CODEN: TETRAB.

AB Sepn. of syn- and anti-isomers of aralkyl alkyl ketoximes and their tosylates was carried out using 1-phenylpropan-2-one and 1- $\alpha$ -naphthylpropan-2-one. With the established configurations, LiAlH<sub>4</sub> redn. of the oximes and their tosylates was performed and the products were analyzed by gas-liq. chromatog. The results clearly indicate that aziridine formation is strongly influenced by the configurations of the oximes and the oxime tosylates used. 23 references.

L17 ANSWER 92 OF 94 CAPLUS COPYRIGHT 1999 ACS

1968:114306 Document No. 68:114306 Aziridine formation by lithium aluminum hydride reduction of oximes. Kotera, Katsumi; Miyazaki, Sadao; Takashi, Hiromi; Okada, Tetsuo; Kitahonoki, Keizo (Shionogi Res. Lab., Shionogi and

Co. Ltd., Osaka, Japan). Tetrahedron, 24(9), 3681-96 (English) 1968. CODEN: TETRAB.

AB Aziridine formation by LiAlH<sub>4</sub> redn. of oximes was extended to compd. types

such as ArCH<sub>2</sub>C(:NOH)R, ArC(:NOH)R, ArCHC(:NOH)R', and ArCH<sub>2</sub>C(:NOH)H. The results were satisfactory for generalization of this reaction. 29 references.

L17 ANSWER 93 OF 94 CAPLUS COPYRIGHT 1999 ACS

1968:95635 Document No. 68:95635 2,6-Methanonaphth[1,2-d]azocines. Perry, Robert L.; Albertson, Noel F. (Sterling-Winthrop Res. Inst., Rensselaer, N. Y., USA). J. Med. Chem., 10(6), 1184-6 (English) 1967. CODEN:

JMCMAR.

GI For diagram(s), see printed CA Issue.

AB Some 2,6-methanonaphth[1,2-d]azocines are prep'd. by the same route used by

May and coworkers (1957) to prep. 2,6-methano-3-benzazocine ring systems. 1,3,4-Trimethylpyridinium iodide is treated with

1-naphthylmethylmagnesium

chloride to give 1,3,4-trimethyl-2-(1-naphthylmethyl)-1,2-dihydropyridine (I), which is reduced with NaBH<sub>4</sub> to the corresponding 1,2,5,6-tetrahydro deriv., which on refluxing with HBr gives a mixt. of cis- and trans-1,2,3,4,5,6-hexahydro-3,6,13-trimethyl-2,6-methanonaphth[1,2-d]azocine (II and III, resp.). II, having 6-quasiequatorial and 13-axial Me groups, is sepd. from III, having 6-quasiequatorial and 13-equatorial Me groups, by recrystn. or chromatog. on SiO<sub>2</sub>. Perchlorination of I gave the perchlorate. Addn. and loss of

HCN

in to the perchlorate according to the 5-step method of Fay (1963) results in

the trans-tetrahydropyridine deriv., which can be cyclized with AlCl<sub>3</sub> to give almost exclusively III. The assignment of configuration of the 6,13-Me groups is based on N.M.R. data. The possibility of cyclization of

the tetrahydro deriv. to the 8-position on the naphthalene ring rather than to the 2-position is excluded on the basis of ir and N.M.R. investigations of acenaphthene, naphthalene-1,8-dicarboxylic acid, 1,8-naphthalenedimethanol, 1,2-dimethylnaphthalene, and 1-chloromethyl-2-methylnaphthalene as model compds. II and III are converted to the norbases with CNBr, the norbases acetylated with cyclopropylcarbonyl chloride, and the N-acyl deriv. reduced with LiAlH<sub>4</sub>

to

the cyclopropylmethyl analog. Similarly prep'd. are the cis-N-cyclobutylmethyl and N-phenethyl derivs. and the trans-N-(3-methyl-2-butenyl) deriv. The naphthazocines are all inactive at doses of 40 mg./kg. i.p. and on the rat tail flick test at doses of

120

mg./kg. s.c. and (or) i.p., with some activity being noted on the inclined

screen which is less than that seen in the benzazocine series. The cyclopropyl Me derivs. have ED<sub>50</sub> values of 55 mg./kg. i.p. and the cyclobutyl Me deriv. of 80 mg./kg. i.p. on the inclined screen.

L17 ANSWER 94 OF 94 CAPLUS COPYRIGHT 1999 ACS

1967:402648 Document No. 67:2648 Stereochemistry of aziridine formation by lithium aluminum hydride reduction of oximes. Kotera, Katsumi; Okada,

Tetsuo; Miyazaki, Sadao (Shionogi Co., Osaka, Japan). Tetrahedron Lett. (9), 841-4 (English) 1967. CODEN: TELEAY.

GI For diagram(s), see printed CA Issue.

AB Pure cryst. anti-1-phenylpropan-2-one oxime (I, 300 mg., m. 62-3.degree.) refluxed 2 hrs. in 10 ml. tetrahydrofuran with 2.2 molar equivs. of LiAlH<sub>4</sub> and the product mixt. analyzed by gas-liquid chromatog. gave 4.7% cis-2-phenyl-3-methylaziridine (II, R = Ph) (III), 18% aziridine (IV, R = Ph) (V) and 65% primary amine RCH<sub>2</sub>CH(NH<sub>2</sub>)Me (VI, R = Ph) (VII). Redn. of 5 .apprx.7:1 anti-syn-I under the same conditions gave 13% III, 13% V, and 56% VII whereas 2 .apprx.3:1 anti-syn-I yielded 23% III, 8.8% V, and 56% VII. The isolation of the pure anti isomer of 1-.alpha.-naphthylpropan-2-one oxime (VIII), m. 96-7.degree., permitted similar redns. The detn. of configurations and the quant. analyses of anti- and syn-VIII were based on the recorded N.M.R. data. Pure anti-VIII (150 mg.) refluxed 3 hrs. in 5 ml. tetrahydrofuran with 75 mg. LiAlH<sub>4</sub> gave 15.2% II (R = .alpha.-C<sub>10</sub>H<sub>7</sub>) (IX), 28.9% IV (R = .alpha.-C<sub>10</sub>H<sub>7</sub>) (X), and 53.5% VI (R = .alpha.-C<sub>10</sub>H<sub>7</sub>) (XI). Similar redn. of 3.6 .apprx.3.8:1 anti-syn-VIII and 1.3 .apprx.1.4:1 anti-syn-VIII gave 26.1, 23.3, 41.1, and 39.0, 15.0, 33.3% yields of IX, X, and XI, resp. Neither of the previously proposed mechanisms (CA 62: 16167e) based on the Neber and closely related rearrangement can reasonably explain the dependence of the products on the configurations of the oximes.

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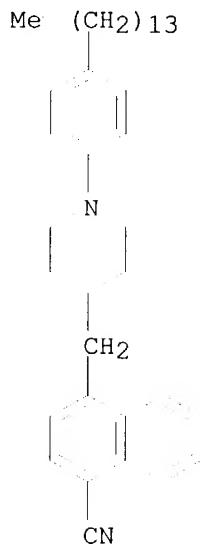
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YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:n

=> d 1 4 7-10 14 18 112

L12 ANSWER 1 OF 209 REGISTRY COPYRIGHT 1999 ACS  
RN 217480-46-1 REGISTRY  
CN 1-Naphthalenecarbonitrile, 4-[(1-(4-tetradecylphenyl)-4-  
piperidinyl)methyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C37 H50 N2

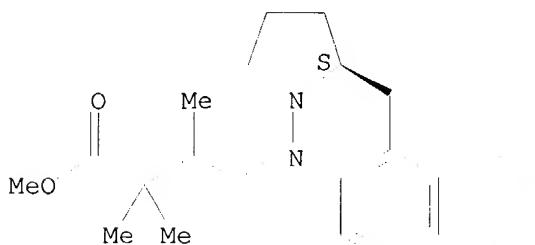
SR CA  
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L12 ANSWER 4 OF 209 REGISTRY COPYRIGHT 1999 ACS  
RN 212504-44-4 REGISTRY  
CN Butanoic acid, 2,2,3-trimethyl-4-[(2S)-2-(1-naphthalenylmethyl)-1-pyrrolidinyl]imino-, methyl ester (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C23 H30 N2 O2  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

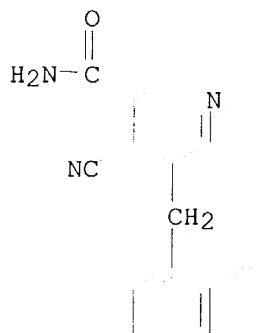
Absolute stereochemistry.  
Double bond geometry unknown.



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

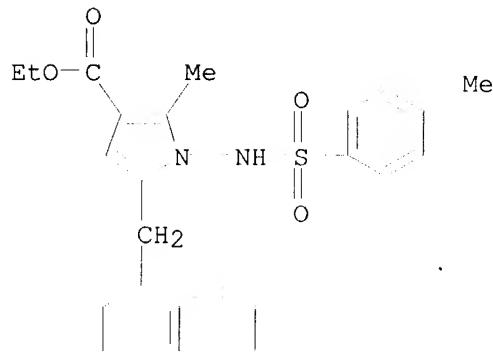
L12 ANSWER 7 OF 209 REGISTRY COPYRIGHT 1999 ACS  
RN 205685-74-1 REGISTRY  
CN 3-Pyridinecarboxamide, 4-cyano-5-(1-naphthalenylmethyl)- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C18 H13 N3 O  
SR CA

LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

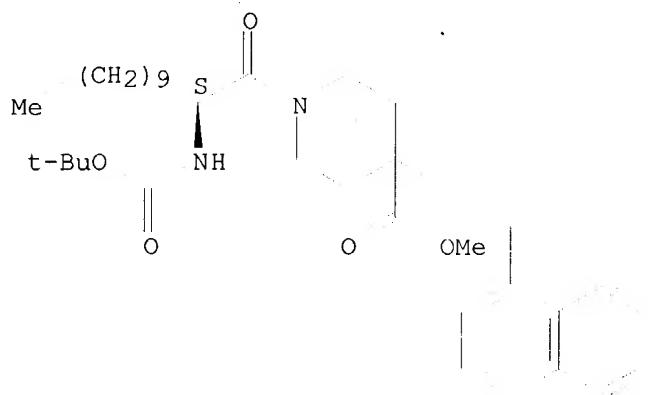
L12 ANSWER 8 OF 209 REGISTRY COPYRIGHT 1999 ACS  
RN 200623-96-7 REGISTRY  
CN 1H-Pyrrole-3-carboxylic acid,  
2-methyl-1-[(4-methylphenyl)sulfonyl]amino]-  
5-(1-naphthalenylmethyl)-, ethyl ester (9CI) (CA INDEX NAME)  
MF C26 H26 N2 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L12 ANSWER 9 OF 209 REGISTRY COPYRIGHT 1999 ACS  
RN 198649-23-9 REGISTRY  
CN 4-Piperidinecarboxylic acid,  
1-[(2-[(1,1-dimethylethoxy)carbonyl]amino)-1-  
oxododecyl]-4-(1-naphthalenylmethyl)-, methyl ester, (S)- (9CI) (CA  
INDEX  
NAME)  
FS STEREOSEARCH  
MF C35 H52 N2 O5  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L12 ANSWER 10 OF 209 REGISTRY COPYRIGHT 1999 ACS  
RN 198647-23-3 REGISTRY

CN 4-Piperidinecarboxylic acid, 1-(2-amino-1-oxododecyl)-4-(1-naphthalenylmethyl)-, methyl ester, (S)-, trifluoroacetate (5:6) (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C30 H44 N2 O3 . 6/5 C2 H F3 O2

SR CA

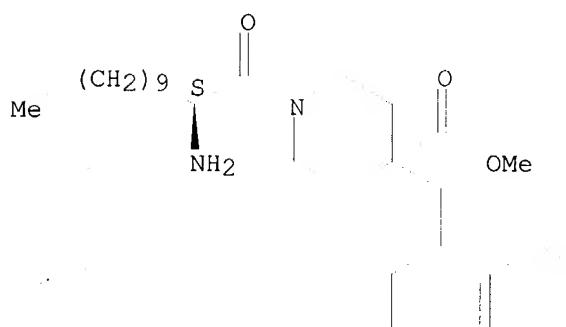
LC STN Files: CA, CAPLUS

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CRN 198647-22-2

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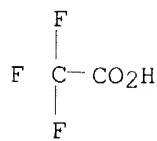
Absolute stereochemistry.



CM 2

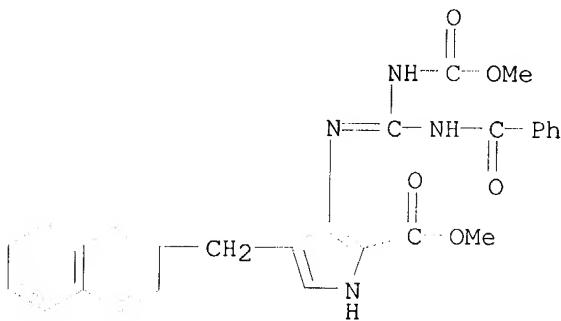
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CMF C2 H F3 O2



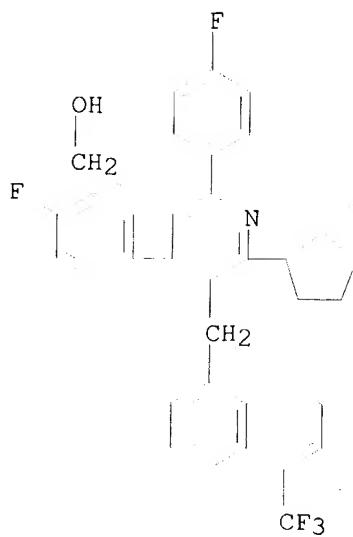
1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L12 ANSWER 14 OF 209 REGISTRY COPYRIGHT 1999 ACS  
 RN 197850-19-4 REGISTRY  
 CN 1H-Pyrrole-2-carboxylic acid,  
 3-[[ (benzoylamino) [(methoxycarbonyl)amino]me  
 thylene]amino]-4-(2-naphthalenylmethyl)-, methyl ester (9CI) (CA INDEX  
 NAME)  
 MF C27 H24 N4 O5  
 SR CA  
 LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L12 ANSWER 18 OF 209 REGISTRY COPYRIGHT 1999 ACS  
 RN 197435-19-1 REGISTRY  
 CN 3-Pyridinemethanol, 6-cyclopentyl-2,4-bis(4-fluorophenyl)-5-[(5-  
 (trifluoromethyl)-1-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C35 H28 F5 N O  
 SR CA  
 LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> d 209 112 ide cbib

L12 ANSWER 209 OF 209 REGISTRY COPYRIGHT 1999 ACS

RN 8076-54-8 REGISTRY

CN Thiourea, N,N'-bis[(4-chlorophenyl)methyl]-, mixt. with  
 1-[4-hydroxy-4-(2-naphthalenylmethyl)-1-octyl-3-piperidinyl]-2-(2-naphthalenyl)ethanone (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Ethanone, 1-[4-hydroxy-4-(2-naphthalenylmethyl)-1-octyl-3-piperidinyl]-2-(2-naphthalenyl)-, mixt. contg. (9CI)

MF C36 H43 N O2 . C15 H14 Cl2 N2 S

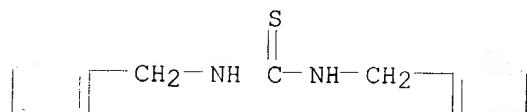
CI MXS

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

CM 1

CRN 57206-73-2

CMF C15 H14 Cl2 N2 S



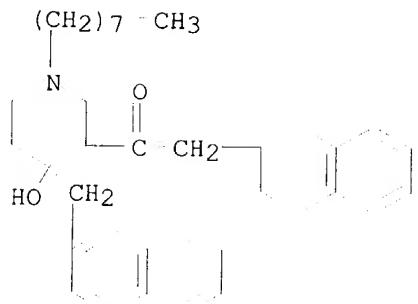
C1

C1

CM 2

CRN 57206-72-1

CMF C36 H43 N O2



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 77:28268 Acidic zinc fluoborate electrolyte for a zinc electroplating process. Page, Walter; Schevey, William R.; Van der Mey, John E. (Allied Chemical Corp.). U.S. US 3655533 19720411, 7 pp. (English). CODEN: USXXAM. APPLICATION: US 70-89068 19701112.

$$\Rightarrow \log y$$

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	45.18	1480.10
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)		SINCE FILE ENTRY
CA SUBSCRIBER PRICE	0.00	-58.37

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